201-15213

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April 29, 2004

The Honorable Michael O. Leavitt, Administrator
U.S. Environmental Protection Agency
PO BOX 1473
Merrifield, VA 22116

Attention: Chemical Right-to-Know
HPV Consortium
Di-Tertiary (C9-C12) Alkyl Polysulfides Category

Dear Administrator Leavitt::

Chevron Phillips Chemical Company LP and ATOFINA Chemicals are pleased to submit High Production Volume (HPV) test plans for Di-Tertiary (C9-C12) Alkyl Polysulfides Category which includes the following:

- Polysulfides, di-tert-nonyl (CAS# 68425-16-1)
- Pentasulfide, di-tert-dodecyl (CAS# 31565-23-8)
- tert-Dodecylmercaptan, sulfur reaction product (CAS# 68583-56-2)
- Polysulfides, di-tert-dodecyl (CAS# 68425-15-0)

Electronic copies of the Test plan and IUCLID dossiers are accompanying this letter via email to the EPA HPV robust summary email address (http://www.epa.gov/chemrtk/srbstsum.htm). This submission is also being sent, via email, to oppt.ncic@epa.gov and chem.rtk@epa.gov.

Dr. Vicente Santa Cruz, Ph.D., is our technical contact and can be reached at 832-813-4787 or by email at santav@cpchem.com .

Sincerely,

Fred Marashi, Ph.D.

Enclosures (3)

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201-15213B1

High Production Volume (HPV) Challenge Program

Di-tertiary (C9-C12) Alkyl Polysulfides Category

Test Plan

CAS Numbers:

68425-16-1

68583-56-2

31565-23-8

68425-15-0

Chevron Phillips Chemical Company LP
10001 Six Pines Drive
The Woodlands, Texas 77380

ATOFINA Chemicals, Inc.
2000 Market Street
19103 Philadelphia, PA

April 2004

EXECUTIVE SUMMARY

Chevron Phillips Chemical Company LP (CPChem) and ATOFINA Chemicals, Inc. (ATOFINA) have jointly volunteered under the Polysulfides Scientific Research Program to assess the health and environmental hazards, including selected physicochemical characteristics, of the Di-Tertiary (C9-C12) Alkyl Polysulfides Category (referred to hereafter as the Category). The Di-Tertiary (C9-C12) Alkyl Polysulfides Category Test Plan is being submitted to fulfill the United States Environmental Protection Agency (USEPA) High Production Volume (HPV) Challenge Program commitment for di-tertiary nonyl polysulfide (CASN 68425-16-1). Other substances in this Category include the Organisation of Economic Cooperation and Development (OECD) listed HPV substance, di-tertiary dodecyl pentasulfide (CASN 31565-23-8) and di-tertiary dodecyl polysulfides (CASN 68583-56-2 and 68425-15-0). All members of this Category exist as a range of mixtures of isomers that are characterized by a common core polysulfide chain that can range from 2 to 8 sulfur atoms in length. These polysulfide chains are terminated with increasingly hydrophobic branched alkyl groups that contain a total of 9 or 12 carbon atoms on each end.

Data from company proprietary files, peer-reviewed literature, and/or calculated endpoints using widely accepted computer modeling programs have been identified for purposes of this program. The summary of available data for the Di-tertiary (C9-C12) Alkyl Polysulfides Category members presents evidence that the members of this Category have similar physical/chemical, environmental, and toxicological properties, and that they follow predictable patterns based upon their chemical composition. Importantly, the Category members are extremely hydrophobic and sorptive, and have very low water solubility and vapor pressure, both of which decrease with increasing carbon number in the tertiary alkyl groups. The hydrophobicity and low water solubility lead to very high predicted Log Kows (>9). These materials will be highly sorptive and tend to form complexes with organic substances in environmental matrices. They are unlikely to be in solution in the environment as free solutes, and therefore have low bioavailability and low predicted bioconcentration factors. They are also of relatively low toxicity to aquatic organisms and mammals.

Limited physiochemical data are available for members of this category, therefore it is proposed to conduct Melting Point (OECD 102), Boiling Point (OECD 103), Vapor Pressure (OECD 104), Partition Coefficient (OECD 117 or 107), and Water Solubility (OECD 105) testing for di-tertiary nonyl polysulfide.

A review of the existing data for the Category shows that sufficient data are available to characterize environmental fate and aquatic toxicity. Environmental fate data for the Category chemicals show that these substances are expected to be stable and resistant to biotic and abiotic degradation mechanisms in the environment, are extremely hydrophobic and sorptive, and have very low water solubility and bioavailability. Ultimately, they will not bioaccumulate, and will partition into soil and sediment compartments when released in the environment. Additionally, acute fish, daphnid, and algal growth inhibition studies were conducted on this Category and no toxicity was observed at the solubility limit.

The considerable existing mammalian toxicity information for the Category demonstrates that these substances share a similar order of toxicity. Mammalian acute toxicity data demonstrates a low order of toxicity via oral, dermal, and inhalation routes of exposure. Genotoxicity data exist for Category members and indicate that genotoxicity is not expected. Repeated dose toxicity testing on di-tertiary-dodecyl pentasulfide (28 day) showed a NOAEL of 250 mg/kg bw and a LOAEL of 1000 mg/kg bw in rats and no further repeated dose toxicity testing is required. No Reproductive Toxicity data were available for any of the Category members. A Developmental Toxicity study

was completed for di-tertiary dodecyl pentasulfide in Sprague-Dawley rats. Both the maternal and teratogen NOAEL were determined to be 1000 mg/kg bw and no clinical signs, unscheduled deaths, abortions, or total resorptions were observed in any group. Likewise, no treatment-related external anomalies or malformations; soft tissue malformations or anomalies; or skeletal malformations, anomalies or variations were observed in any group.

The majority of HPV endpoints have been satisfied for the USEPA HPV Challenge Program. Testing is proposed for the following endpoints for di-tertiary nonyl polysulfide:

- Melting Point
- Boiling Point
- Vapor Pressure
- Partition Coefficient
- Water Solubility
- Reproductive Toxicity (90-day Subchronic with reproductive endpoints)

In addition, there were insufficient data to fulfill the Reproductive Toxicity endpoint and therefore, testing is proposed. According to the annex VII of the proposal (dated 29.10.2003) for a regulation of the European parliament and of the council concerning the Registration, Evaluation, Authorisation and Restrictions of chemicals (REACH), an additional standard information requirement for substances manufactured or imported in quantities of 100 tonnes or more should be a sub-chronic toxicity study (90-day) (Commission of the European Communities [EC], 2003). In order to meet future ICCA and REACH testing requirements and to eliminate unnecessary and/or duplicate testing, the Polysulfides Scientific Research Program proposes to perform a Sub-chronic Oral Toxicity – Rodent 90-day Study (OECD 408) with a focus on reproductive endpoints. This study, in combination with the existing Developmental Toxicity study, will fulfill the Reproductive Toxicity endpoint. Current EPA and OECD guidance states that "When a 90-day repeated dose study is available and is sufficiently documented with respect to studying effects on the reproductive organs, and a developmental study is available, the requirements for the reproductive toxicity endpoints are satisfied" (USEPA, 1998; OECD 2002). Di-tertiary nonyl polysulfide is recommended for this test because of its lower molecular weight (and is therefore incrementally less hydrophobic) and represents a potentially more bioavailable fraction of the Di-tertiary (C9-C12) Alkyl Polysulfides Category.

The following table summarizes the available data for the Di-tertiary (C9-C12) Alkyl Polysulfides:

Matrix of Available and Adequate Data on Di-tertiary (C9-C12) Alkyl polysulfides Category

"SIDS ENDPOINT"	di-tertiary nonyl polysulfide US HPV SUBSTANCE Y/N	di-tertiary dodecyl polysulfide & di-tertiary dodecyl pentasulfide Y/N	Testing Planned? Y/N
Physical and Chemical Data			
Melting Point	N	Y	Y (nonyl)
Boiling Point	N	Y	Y (nonyl)
Vapor Pressure	N	Y	Y (nonyl)
Partition Coefficient	N	Y	Y (nonyl)
Water Solubility	N	Y	Y (nonyl)

Environmental Fate and Pathways			
Photodegradation	Y	Y	N
Stability in Water (Hydrolysis)	NA	NA	NA
Transport/Distribution	Y	Y	N
Biodegradation	Y	Y	N
Ecotoxicity			
Acute/Prolonged Toxicity to Fish	Y	N	N
Acute Toxicity to Aquatic Invertebrates (*Daphnia*)	N	Y	N
Acute Toxicity to Aquatic Plants (Algae)	N	Y	N
Toxicity			
Acute Toxicity (Oral)	Y	Y	N
Acute Toxicity (Dermal)	N	Y	N
Acute Toxicity (Inhalation)	Y	N	N
Repeated Dose	N	Y	N
GeneticToxicity *in vitro* – Gene Mutation	Y	Y	N
Genetic Toxicity *in vitro* – Chromosomal Aberration	Y	Y	N
Reproductive Toxicity	N	N	Y (nonyl)
Developmental Toxicity	N	Y	N

NA = not applicable

Note: **The data used to characterize the OECD SIDS endpoints for substances in this Test Plan were identified either in company proprietary files, peer-reviewed literature, and/or calculated using widely accepted computer modelling programs. All data were evaluated for study reliability in accordance with criteria outlined by the USEPA (1999a). Only studies that met the reliability criteria of "1" (reliable without restrictions) or "2" (reliable with restrictions) were used to fulfil OECD SIDS endpoints. Additional data for substances in this Category are also included in the IUCLID (International Uniform Chemical Information Dataset) attached in Annexes I and II. A more detailed discussion of the data quality and reliability assessment process used to develop this test plan is provided in Annex III.**

CONTENTS

Tables

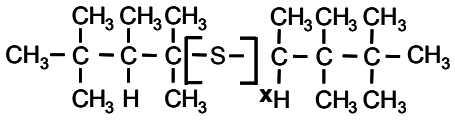
1 IDENTITY

1.1 Identification of the Substance

The Di-tertiary (C9-C12) Alkyl Polysulfides Category consists of the United States Environmental Protection Agency (USEPA) High Production Volume (HPV) listed substance, di-tertiary nonyl polysulfide (CAS # 68425-16-1); the Organisation of Economic Cooperation and Development (OECD) HPV listed substance, di-tertiary dodecyl pentasulfide (CAS Number 31565-23-8); and di-tertiary dodecyl polysulfides (CAS Number 68583-56-2 and 68425-15-0). Due to their close structural similarity, these compounds comprise the proposed Di-tertiary (C9-C12) Alkyl Polysulfides Category for the purpose of meeting the requirements of the US HPV Challenge Program and the International Council of Chemical Associations (ICCA) HPV Initiative.

In general, these dialkyl polysulfides exist as complex mixtures of isomers with varying distributions of alkyl chain length and tertiary branching, and sulfur atom chain length. All members of this Category exist as a range of mixtures of isomers that are characterized by a common core polysulfide chain that can range from 2 to 8 sulfur atoms in length. These polysulfide chains are terminated with increasingly hydrophobic branched alkyl groups that contain a total of 9 or 12 carbon atoms on each end.

1.1.1 Di-Tertiary-Nonyl Polysulfide

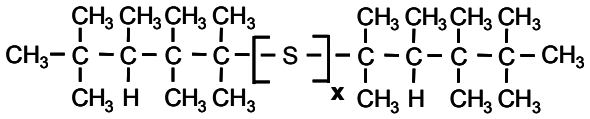
CAS Number:	68425-16-1
EINECS Number	270-336-2
IUPAC Name:	
EINECS Substance Name:	Polysulfides, di-tert-nonyl
Molecular Formula:	$C_{18}H_{38}S_X$
Structural Formula:	
	Where **x** = 2-5, predominantly 3
Molecular Weight:	~ 350
Synonyms:	TPS 37; TNPS; t-Nonyl polysulfide; tertiary-Nonyl polysulfide

1.1.2 Di-Tertiary-Dodecyl Polysulfide

CAS Number:	68583-56-2 / 68425-15-0
EINECS Number	271-518-4 / 270-335-7
IUPAC Name:	
EINECS Substance Name:	Tert-Dodecanethiol, sulfurized / Polysulfides, di-tert-dodecyl

Molecular Formula: $C_{24}H_{50}S_X$

Structural Formula:

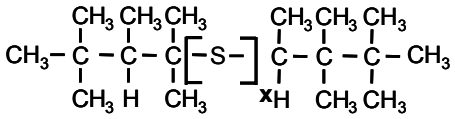


Where **x** = 2-8, predominantly 3-5

Molecular Weight: ~ 498
Synonyms: TDPS 320; t-Dodecyl polysulfide; tertiary-Dodecyl polysulfide; Di-t-dodecyl polysulfide; t-Dodecyl mercaptan, sulfurized; Di-tertiary dodecyl polysulfide (3S); tert-Dodecanethiol, sulfurized

1.1.3 Di-Tertiary Dodecyl Pentasulfide

CAS Number: 31565-23-8
EINECS Number 250-702-8
IUPAC Name:
EINECS Substance Name: Di(tert-dodecyl) pentasulphide
Molecular Formula: $C_{24}H_{50}S_X$
Structural Formula:



Where **x** = 5

Molecular Weight: ~ 498
Synonyms:

1.2 Purity/Impurities/Additives

1.2.1 Di-Tertiary-Nonyl Polysulfide

Purity: 100%
Main impurities**:** none

1.2.2 Di-Tertiary-Dodecyl Polysulfide and Di-Tertiary Dodecyl Pentasulfide

Purity: 100%
Main impurities**:** none

1.3 Physico-Chemical properties

Physico-chemical data for the Category chemicals were either tested or estimated using EPIWIN© (USEPA, 2000) and are provided in the following table.

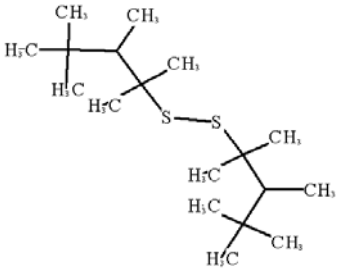
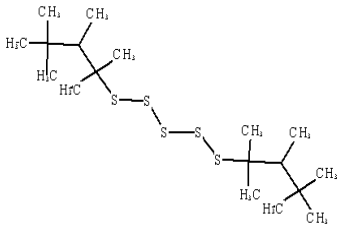
Table 1. Summary of Physical and Chemical Properties (Measured [M] and Calculated [C])

Test	M/C	di-tertiary nonyl polysulfide	M/C	di-tertiary dodecyl pentasulfide
Physical state	-	yellow to yellow-orange liquid		yellow to yellow-orange liquid
Odor	-	Mildly unpleasant		mildly unpleasant
Melting Point	-	ND	M[1]	< 0 °C
	C[2]	96.70 °C	C[2]	178.66 °C
Boiling Point	-	ND	M[1]	> 200 ºC at 1013 hPa
	C[2]	350.6 ºC	C[2]	463.57 ºC
Relative Density		ND		ND
Vapor Pressure	-	ND	M[1]	<0.03 hPa at 20 ºC
	C[2]	3.43 x10^{-5} hPa at 25 ºC	C[2]	7.6 x10^{-9} hPa at 25 ºC
Water Solubility	-	ND	M[1]	Not soluble
	C[3]	9.612 x10^{-5} mg/L	C[3]	5.368 x10^{-8} mg/L
Partition coefficient n-octanol/water (log value)	-	ND	C[4]	> 5
	C[5]	9.14	C[5]	11.86
Henry's Law Constant	C[6]	0.174 atm-m^3/mol at 25°C	C[6]	2.27 atm-m^3/mol at 25°C
Organic Carbon/Water Partition Coefficient (Log Koc)	C[7]	2.8 x 10^5	C[7]	1.9 x 10^7
Flammability	M[8]	Slight flammability Flash point 145°C (PMCC, ASTM D93)	M[8]	Slight flammability Flash point 132°C (PMCC, ASTM D93)

[1] Source: Atofina, 2003
[2] EPIWIN v3.10; calculated using MPBPWIN v1.40 (determined at 760 mmHg)
[3] EPIWIN v3.10; calculated using WSKOW v1.40
[4] Source: Atofina, 2003
[5] EPIWIN v3.10; calculated using KOWWIN v1.66
[6] EPIWIN v3.10; calculated using HENRYWIN v3.10
[7] EPIWIN v3.10; calculated using PCKOC v1.66
[8] Source: CPChem MSDS
ND = No Data Available

For additional perspective, Table 1a provides EPIWIN data developed for representative polysulfide structures containing 2 and 5 sulfurs.

Table 1a. EPIWIN Physicochemical Data for Representative Structures

Physical and Chemical Data		
Parameter	 (C_{18} H_{38} S_2)	 (C_{18} H_{38} S_5)
Melting Point	69.03 ºC [1]	143.65 ºC[1]
Boiling Point	314.76 ºC [1]	417.14 ºC[1]
Vapor Pressure	0.000342 mmHg at 25 ºC [1]	2 x 10^{-7} mmHg at 25 ºC [1]
Kow Partition Coefficient	9.14 [2]	9.14 [2]
Water Solubility	1.495 x 10^{-4} mg/L at 25 ºC [2]	3.881 x 10^{-5} mg/L at 25 ºC [2]

[1]EPIWIN v3.10; MPBPWIN v1.40.
[2]EPIWIN v3.10; calculated using WSKOW v1.40.

Conclusion

Limited physiochemical data are available for members of the Category and the Polysulfides Scientific Research Program therefore proposes to complete the following testing for di-tertiary nonyl polysulfide:

- Melting Point (OECD Guideline 102, "Melting Point/Melting Range")
- Boiling Point (OECD Guideline 103, "Boiling Point")
- Vapor Pressure (OECD Guideline 104, "Vapour Pressure")
- Partition Coefficient – (OECD Guideline 117 "Partition Coefficient (n-octanol/water), High Performance Liquid Chromatography (HPLC) Method" – Note: In general, calculated values greater than 6 are recognized to not be reliable and therefore, testing is required following either OECD Guideline 107 or 117. According to OECD guidelines, a high log Kow cannot be correctly determined using the OECD 107 (shake flask method). As a result, the OECD guideline 117 (HPLC method) is indicated. However, due to the expected low solution concentrations and the test material not being UV active, a non-specific HPLC method such as HPLC/UV or HPLC/Refractive Index, may not be possible, rather, HPLC with Radiochemical detection or HPLC/Mass Spectrometry detection may be recommended depending on sample availability and the results of preliminary studies.
- Water Solubility (OECD Guideline 105, "Water Solubility")

1.4 Category Justification

A chemical category is defined as a group of chemicals whose physicochemical and toxicological properties are likely to be similar to or follow a regular pattern as a result of structural similarity (USEPA, 1999a). The Polysulfides Scientific Research Program has evaluated the dialkyl polysulfides in this Test Plan with this guidance in mind, and has opted to form the Di-tertiary (C9-C12) Alkyl Polysulfides Category.

Common Dialkyl Polysulfide Structures and Functional Groups

In general, these dialkyl polysulfides exist as complex mixtures of isomers with varying distributions of alkyl chain length and tertiary branching, and sulfur atom chain length. All members of this Category exist as a range of mixtures of isomers that are characterized by a common core polysulfide chain that can range from 2 to 8 sulfur atoms in length. These polysulfide chains are terminated with increasingly hydrophobic branched alkyl groups that contain a total of 9 or 12 carbon atoms on each end.

GENERAL ALKYL POLYSULFIDE STRUCTURE $R—S_x—R'$	• Sulfur atom chains form the core of the molecule and range from 2 to 8 sulfurs in length. • R = highly methyl branched alkyl groups containing 9 or 12 carbons each and which terminate at the core sulfur atom chains

Similar or Even Identical Properties or Hazards

The summary of available data for the Di-tertiary (C9-C12) Alkyl Polysulfides Category members presents evidence that the members of this Category have similar physical/chemical, environmental, and toxicological properties, and that they follow predictable patterns based upon their chemical composition. Importantly, the Category members are extremely hydrophobic and sorptive, and have very low water solubility and vapor pressure, both of which decrease with increasing carbon number in the tertiary alkyl groups. The hydrophobicity and low water solubility lead to very high predicted Log Kows (>9). These materials will be highly sorptive and tend to form complexes with organic substances in environmental matrices. They are unlikely to be in solution in the environment as free solutes, and therefore have low bioavailability and low predicted bioconcentration factors. They are also of relatively low toxicity to aquatic organisms and mammals.

GENERAL INFORMATION ON EXPOSURE

1.5 Production Volumes and Use Pattern

1.5.1 Manufacturers:

- Chevron Phillips Chemical Company LP (CPChem)
- ATOFINA Chemicals, Inc.

1.5.2 Use Pattern:

The principal uses of polysulfides are as reagents for catalyst sulfidation in metalworking and metal processing industries. These sulphide reagents improve initial catalyst activity and lengthen production cycles for nickel, molybdenum, cobalt, and tungsten hydrotreating catalysts.

Polysulfides are also commonly used in the metal working, steel rolling, and wire drawing industries in the formulation of lubricant additives to improve equipment functionality at extreme pressures. The sulphur reacts with the metal under extreme heat and pressure to form a metal sulphide layer that allows for slippage and movement and reduces friction and damage to metal equipment.

Tert-nonyl polysulfide and tert-dodecyl polysulfide are used in general metalworking applications. Tert-dodecyl polysulfide is also used in steel rolling oils and non-ferrous metalworking applications. Tert-butyl polysulfide can be used as a replacement for sulfurized isobutylene for gear oil lubricants.

1.6 Environmental Exposure and Fate

The weight of evidence indicates that no further environmental fate testing is necessary to meet HPV SIDS endpoints for the Di-tertiary (C9-C12) Alkyl Polysulfides Category. Environmental fate data for the Category chemicals were either tested or estimated using EPIWIN and are provided in the following sections. Overall, these substances are expected to be stable and resistant to biotic and abiotic degradation mechanisms in the environment, are extremely hydrophobic and sorptive, and have very low water solubility and bioavailability. Ultimately they will not bioaccumulate, and will partition into soil and sediment compartments when released to the environment.

1.6.1 Sources of Environmental Exposure

1.6.2 Photodegradation

Values for atmospheric oxidation were calculated based upon the representative chemical structures for this Category using EPIWIN. No reaction with ozone could be estimated due to lack of suitable labile functional groups. These results demonstrate that substances in this Category are similar in estimated atmospheric stability or reactivity.

Table 2. Photodegradation and Atmospheric Oxidation Data.

Test	di-tertiary nonyl polysulfide	di-tertiary dodecyl pentasulfide
OH Half-Life	0.023 Days	0.016 Days
OH Rate Constant	473 $x10^{-12}$ cm^3/molecule-sec	683 $x10^{-12}$ cm^3/molecule-sec

Source: EPIWIN v3.10; calculated using AOP Program v1.90

1.6.3 Stability in Water

EPIWIN was unable to calculate a hydrolysis rate for any of the polysulfides (di-tertiary dodecyl or di-tertiary nonyl) due to the absence of functional groups that are labile to hydrolysis. Given the very low water solubility of these materials and the lack of a functional group to hydrolyze, further testing for hydrolytic stability is not warranted.

1.6.4 Transport between Environmental Compartments

Fugacity modeling for the Category and representative di-tertiary nonyl polysulfide structures (S2 and S5) members using EPIWIN (v3.10) produced the following results for di-tertiary-nonyl polysulfide:

Table 3. Fugacity Results for Di-tertiary Nonyl Polysulfide

Compartment	100% to air	100% to water	100% to soil	Equally to each compartment
Air	75%	0.0%	0.0%	0.00474%
Water	0.0745%	1.87%	0.0021%	1.28%
Soil	21%	0.0%	99.9%	31.6%
Sediment	3.91%	98.1%	0.11%	67.1%

for di-tertiary-dodecyl pentasulfide:

Table 4. Fugacity Results for Di-tertiary Dodecyl Polysulfide

Compartment	100% to air	100% to water	100% to soil	Equally to each compartment
Air	4.35%	0.0%	0.0%	0.00323%
Water	0.346%	1.87%	0.0021%	1.27%
Soil	77.1%	0.0%	99.9%	31.9%
Sediment	18.2%	98.1%	0.11%	66.9%

Results are similar and show ultimate partitioning to soil and sediments where these substances will likely be tightly bound to organic phases and unavailable to exert toxicity. Predictably, there is a difference for releases directly to air, where the lower molecular weight di-tertiary nonyl polysulfide Category member is predicted to be slower to partition from the air into the soil compartment. Overall, these data are of adequate quality, and no further fugacity modeling is warranted for this Category.

1.6.5 Biodegradation

The members of this Category have both been tested in European Economic Community/Organisation for Economic Co-operation and Development (EEC/OECD) Ready Biodegradation tests (OECD 301D – Closed Bottle Test) that show no biodegradation for either di-tertiary nonyl polysulfide or di-tertiary dodecyl pentasulfide. These experiments are consistent with EPIWIN, where this Category is predicted not to quickly biodegrade. This is to be expected, given the highly branched nature of the carbon chains. These data are considered valid without restriction, and further Ready Biodegradability testing will not add additional value for this Category.

Table 5. Biodegradation Data.

Test	di-tertiary nonyl polysulfide	di-tertiary dodecyl pentasulfide
Biodegradation	0 in 28 days (non-biodegradable)	0 in 28 days (non-biodegradable)

Source: Atofina, 2003.

1.6.6 Bioaccumulation

The predicted bioconcentration factor (BCF) is low for this Category, suggesting no bioaccumulation hazard. There are 18 to 24 carbon atoms per molecule in the representative molecules used in the modeling of this Category in EPIWIN. The predicted Log Kows for this Category are, therefore, very high, reflecting the very low water solubility and high hydrophobicity of these materials. The predicted organic carbon partition coefficient shows that these materials will be highly sorptive. This also translates into a low predicted fish BCF since these materials will not be bioavailable in the environment due to the combination of low water solubility and tendency to adsorb to surfaces and other hydrophobic constituents in the environment.

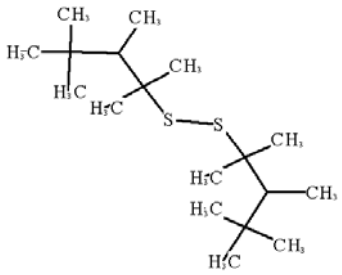
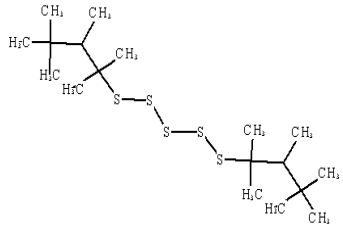
Table 6. Bioaccumulation Data

Test	di-tertiary nonyl polysulfide	di-tertiary dodecyl pentasulfide
Estimated BCF	75.66	3.162

Source: EPIWIN v3.10; calculated using BCF Program v2.14.

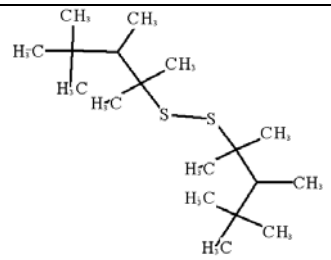
For additional perspective, two additional polysulfides, one containing 2 sulfurs and one containing 5 sulfurs, were run in EPIWIN and the following environmental fate and pathways data were obtained:

Table 6a. Related Structures EPIWIN Environmental Fate and Pathways Data

Environmental Fate and Pathways		
Parameter	 (C_{18} H_{38} S_2)	 (C_{18} H_{38} S_5)
Photodegradation & Atmos. Oxidation: • OH Rate Constant • OH Half Life	232.8774 x 10^{-12} cm^3/molecule-sec[1] 0.551 Hrs[1]	682.8774 x 10^{-12} cm^3/molecule-sec[1] 11.277 Min[1]
Transport/ Distribution Fugacity Estimated Koc: Estimated BCF:	 See Table 6b. 1.418 x 10^5 [(2)] 75.66[3]	 See Table 6b. 8.9 x 10^5 [(2)] 75.66[3]

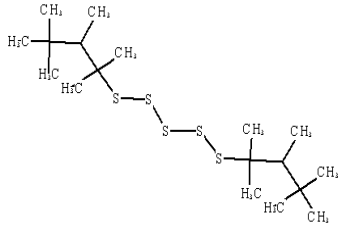
[1]EPIWIN v3.10; calculated using AOP Program v1.90.
[2]EPIWIN v3.10; calculated using PCKOC Program v1.66.
[3]EPIWIN v3.10; calculated using BCF Program v2.14.

Table 6b. EPIWIN Level III Fugacity Results for Representative Structures



(C_{18} H_{38} S_2)

Compartment	100% to air	100% to water	100% to soil	Equally to each compartment
Air	85.7%	0.00%	0.00%	0.00955%
Water	0.0388%	1.87%	0.0021%	1.28%
Soil	12.2%	0.00%	99.9%	31.6%
Sediment	2.03%	98.1%	0.11%	67.1%



(C_{18} H_{38} S_5)

Compartment	100% to air	100% to water	100% to soil	Equally to each compartment
Air	22.0%	0.00%	0.00%	0.00328%
Water	0.277%	1.87%	0.0021%	1.28%
Soil	63.2%	0.00%	99.9%	31.7%
Sediment	14.5%	98.1%	0.11%	67.0%

2 HUMAN HEALTH HAZARDS

2.1 Effects on Human Health

2.1.1 Acute Toxicity

Acute toxicity studies via oral, dermal, and inhalation routes for this Category have been conducted according to relevant OECD/EEC guidelines or methods comparable to those guidelines.

Studies in Animals

Inhalation

An acute study using di-tertiary-nonyl polysulfide was performed on Sprague-Dawley rats using methods comparable to OECD Guideline 403. This study featured exposure to a nominal

concentration of 15.5 mg/l (g/m^3) di-tertiary-nonyl polysulfide and fulfills the requirements for a critical study for this SIDS endpoint. Adequate data are available for this endpoint, and no additional testing is proposed (see Table 7 and IUCLID documents).

Table 7. Acute Toxicity – Results of Inhalation Studies in Animals

Test	di-tertiary nonyl polysulfide	di-tertiary dodecyl pentasulfide
Acute Inhalation	LC_{50} = >15.5 mg/L	No Data Available

Source: Atofina, 2003.

Dermal

Acute dermal toxicity of di-tertiary dodecyl pentasulfide was evaluated in a GLP study performed using Sprague-Dawley rats according to OECD Guideline 402 (Acute Dermal Toxicity). Fourteen days following administration of the test substance there was no evidence of lesion (erythema or oedema), mortality, or behavioral anomaly. This study fulfills the requirements for a critical study for this SIDS endpoint and no additional testing is proposed (see Table 8 and IUCLID documents).

Table 8. Acute Toxicity – Results of Dermal Studies in Animals

Test	di-tertiary nonyl polysulfide	di-tertiary dodecyl pentasulfide
Acute Dermal	No Data Available	$LD_0 \geq$ 2000 mg/kg bw

Source: Atofina, 2003.

Oral

Valid acute oral toxicity studies have been performed for this Category, which show mortality at high doses. These studies fulfill the requirements for a critical study for this SIDS endpoint and no additional testing is proposed (see Table 9 and IUCLID documents).

Table 9. Acute Toxicity – Results of Oral Studies in Animals

Test	di-tertiary nonyl polysulfide	di-tertiary dodecyl pentasulfide
Acute Oral	LD_{50} = 17781 – 21495 mg/kg bw	LD_0 = 12625 mg/kg bw

Source: Atofina, 2003.

Other Routes of Exposure

An acute study using di-tertiary-nonyl polysulfide was performed on Sprague-Dawley rats via intraperitoneal (i.p.) exposure. This study featured exposure to 3350 – 4375 mg/kg body weight di-tertiary-nonyl polysulfide and measurement of behavioral endpoints. Adequate data are available for this endpoint, and no additional testing is proposed (see Table 10 and IUCLID documents).

Table 10. Acute Toxicity – Results of Other Studies in Animals

Test	di-tertiary nonyl polysulfide	di-tertiary dodecyl pentasulfide
Acute Toxicity (i.p.)	LD_{50} = 3350 – 4375 mg/kg bw	No Data Available

Source: Atofina, 2003.

Conclusion

The collective data for the Di-tertiary (C9-C12) Alkyl Polysulfides Category fulfill the requirements for the acute toxicity endpoints. As a result, no additional testing is proposed for purposes of the HPV program (see Tables 7 to 10 and IUCLID documents).

2.1.2 Irritation

Skin Irritation

Studies in Animals

Several valid irritation studies have been performed for the Polysulfides in this Category, all of which show polysulfides to be mild to non-irritants (see Table 11 and IUCLID documents).

Table 11. Irritation – Results of Skin Irritation Studies in Animals

Test	di-tertiary-nonyl polysulfide	di-tertiary dodecyl pentasulfide
Skin Irritation	Slightly Irritating	Slightly irritating

Source: Atofina, 2003.

- Di-tertiary nonyl polysulfide – In a rabbit skin irritation test (undiluted, 24 hours, occlusive), the Primary Dermal Irritation Index (PDII) was 1.88. Di-tertiary nonyl polysulfide was slightly irritating.
- Di-tertiary dodecyl pentasulfide – In a rabbit skin irritation test following OECD Guideline 404, (undiluted, 4 hours, semiocclusive), di-tertiary dodecyl pentasulfide produced a slight erythema in one rabbit and a moderate erythema in 5 rabbits. A slight edema was observed in 3 rabbits. The mean score (24 + 48 + 72 h) for erythema was 1.72 and for edema was 0.39 and di-tertiary dodecyl pentasulfide was slightly irritating.

Eye Irritation

Studies in Animals

Several valid irritation studies have been performed for the Polysulfides Category, all of which show polysulfides to be non-irritants (see Table 12 and IUCLID documents).

Table 12. Irritation – Results of Eye Irritation Studies in Animals

Test	di-tertiary-nonyl polysulfide	di-tertiary dodecyl pentasulfide
Eye Irritation	Slightly irritating	Slightly irritating

Source: Atofina, 2003.

- Di-tertiary nonyl polysulfide – In a rabbit eye irritation test (undiluted, 24 hours, not rinsed), di-tertiary nonyl polysulfide was slightly irritating.
- Di-tertiary dodecyl pentasulfide – In a rabbit eye irritation test following OECD Guideline 405, (undiluted, 24 hours, not rinsed), di-tertiary dodecyl pentasulfide induced a slight chemosis and/or enanthema which persisted for up to 72 hours in 2 animals. Slight iridal congestion was observed up to 48 hours in some animals. The mean score (24 + 48 + 72 h) for chemosis was 0.89; for enanthema was 0.61; for iris was 0.33; and for cornea was 0.00. Di-tertiary dodecyl pentasulfide was slightly irritating.

Conclusion

Several valid skin and eye irritation studies have been performed for the Di-tertiary (C9-C12) Alkyl Polysulfides Category, all of which show polysulfides to be mild to non-irritants. (see Tables 11 and 12 and IUCLID documents).

2.1.3 Sensitisation

Studies in Animals

Skin

Several valid sensitisation studies have been performed for the Polysulfides Category. Data for di-tertiary nonyl polysulfide and di-tertiary dodecyl pentasulfide show ambiguous results, with both positive and negative results being reported. (see Table 13 and IUCLID documents).

Table 13. Sensitisation – Results of Skin Sensitisation Studies in Animals

Test	di-tertiary-nonyl polysulfide	di-tertiary dodecyl pentasulfide
Sensitization	1. Not sensitizing (Guinea pig maximization)	Not sensitizing (ambiguous results)

Source: Atofina, 2003.

- Di-tertiary nonyl polysulfide
    - In a Guinea Pig Maximization test following Directive 96/54/EC, B.6, no cutaneous reactions were observed after the challenge application. According to the maximization method of Magnusson and Kligman, di-tertiary nonyl polysulfide did not induce delayed contact hypersensitivity in guinea pigs.

- Di-tertiary dodecyl pentasulfide – In a Guinea Pig Maximization test following OECD Guideline 406, di-tertiary dodecyl pentasulfide was classified as "not sensitising." However, from the macroscopic and histological results obtained under the experimental conditions, it was concluded that the test article had provoked an aspecific reaction of irritation of weak intensity in 4 out of the 20 treated guinea-pigs. This phenomenon can hide possible weak reactions of cutaneous sensitisation.

Conclusion

Several valid sensitisation studies have been performed for the Di-tertiary (C9-C12) Alkyl Polysulfides Category (see Table 13 and IUCLID documents).

2.1.4 Repeated Dose Toxicity

Studies in Animals

Oral

For this Category, a GLP 28-day subchronic repeated dose study was performed on rats according to EEC guidelines using di-tertiary-dodecyl pentasulfide. This study featured gavage dosing, measurement of mortality, body weight changes, food consumption, hematological and blood biochemical examinations, urinalysis, and organ weights and fulfills the USEPA HPV requirements for this SIDS endpoint. Results from this study showed no deaths related to the treatment during the treatment period or the recovery period. Ptyalism was observed in all the animals of both sexes given 1000 mg/kg/day during the treatment period. During the recovery period no clinical signs were observed. No abnormalities of toxicological importance were noted among hematological and blood biochemical parameters, urinalysis, organ weights, or macro- and microscopic examinations.

An 8-day repeated dose study with rats gavaged with di-tertiary-dodecyl pentasulfide was also completed. No mortality occurred during the treatment period and ptyalism was observed in all the males given 1250 or 2500 mg/kg/day and in 2/4 or 3/4 females given 1250 or 2500 mg/kg/day, respectively. . A slightly lower mean food consumption and body weight gain was observed in the males given 2500 mg/kg/day. A thickened and/or translucent wall of the forestomach was noted for 3/4 females given 2500 mg/kg/day. This study reported NOAEL and LOAEL values similar to those of the longer subchronic repeated dose study and further supports the results of that study.

Table 14. Repeated Dose Toxicity – Results of Oral Studies in Animals

Test	di-tertiary nonyl polysulfide	di-tertiary dodecyl pentasulfide
Repeated Dose (28 Day and 8 Day)	No Data Available	1. 28-Day Rat Oral Gavage Study: No Observed Adverse Effect Levels (NOAEL) =1000 mg/kg bw
		2. 8 Day Rat Oral Gavage Study: NOAEL =1250 mg/kg bw (based on a lower body weight gain in males at 2500 mg/kg) LOAEL = 2500 mg/kg bw

Source: Atofina, 2003.

Conclusion

Adequate data are available for the Di-tertiary (C9-C12) Alkyl Polysulfides Category for this endpoint, and no additional testing is proposed for purposes of the HPV program (see Table 14 and IUCLID documents).

2.1.5 Mutagenicity

Studies in Animals

In vitro Studies

Several valid *in vitro* genetic toxicity/mutagenicity studies have been performed for the Polysulfides Category, all which show no mutagenic activity.

Table 15. Mutagenicity – Results of *In vitro* Studies in Animals

Test	di-tertiary nonyl polysulfide	di-tertiary dodecyl pentasulfide
Genetic – Gene Mutation	Negative with and without activation	Negative with and without activation
Genetic – Chromosomal Aberration	Negative with and without activation	Negative with and without activation

Source: Atofina, 2003.

Conclusion

Adequate data are available for the Di-tertiary (C9-C12) Alkyl Polysulfides Category for this endpoint which indicate that these materials are not mutagenic. No additional testing is proposed for purposes of the HPV program (see Table 15 and IUCLID documents).

2.1.6 Toxicity for Reproduction

No reproduction toxicity data were available for any of the Category members. Therefore, testing to fulfill the Reproductive Toxicity endpoint is proposed.

The Subchronic Oral Toxicity – Rodent 90-day Study (OECD 408) with a focus on reproductive endpoints is proposed, which in combination with the Developmental Toxicity study will fulfill the Reproductive Toxicity endpoint. Current EPA and OECD guidance states that "When a 90-day repeated dose study is available and demonstrates no effect on reproductive organs, in particular the testes, then a developmental study (e.g. OECD Test guidelines 414) can be considered as an adequate test to complete information on reproduction/developmental effect" (USEPA, 1998; OECD, 2002). The 90-Day Subchronic study was chosen by the Polysulfides Scientific Research Program in order to meet future ICCA and REACH[1] testing requirements and to eliminate unnecessary and/or duplicate testing. Di-tertiary nonyl polysulfide is recommended for this test because of its lower molecular weight (and is therefore incrementally less hydrophobic) and represents a potentially more bioavailable fraction of the Di-tertiary (C9-C12) Alkyl Polysulfides Category.

Studies in Animals

Effects on Fertility

No data available.

Developmental Toxicity

A Developmental Toxicity test was completed for di-tertiary dodecyl pentasulfide in Sprague-Dawley rats following OECD Guideline 414 "Teratogenicity." No clinical signs, no unscheduled deaths, no abortions or total resorptions were observed in any group. The food consumption and body weight gain of the pregnant females from all treated groups were similar to those of controls. No treatment-related macroscopic findings were observed in any group. In the 1000 mg/kg/day group, a slightly increased post-implantation loss (represented mainly by late resorptions in one female) was observed, however, it could not be demonstrated that this single event was related to treatment. No treatment-related effects were observed on the number of live fetuses per animal, the fetal body weight, or the sex ratio. Likewise, no treatment-related external anomalies or malformations; soft tissue malformations or anomalies; or skeletal malformations, anomalies or variations were observed in any group.

Table 16. Toxicity for Reproduction – Results of Developmental Toxicity Studies in Animals

Test	di-tertiary nonyl polysulfide	di-tertiary dodecyl pentasulfide
Developmental/ Teratogenicity	No Data Available	NOAEL maternal tox. = 1000 mg/kg bw NOAEL teratogen = 1000 mg/kg bw

Source: Atofina, 2003.

[1] According to the annex VII of the proposal (dated 29.10.2003) for a regulation of the European parliament and of the council concerning the Registration, Evaluation, Authorisation and Restrictions of chemicals (REACH), establishing a European chemicals agency and amending directive 1999/45/EC and regulation (EC) {on persistent organic pollutants}, an additional standard information requirements for substances manufactured or imported in quantities of 100 tonnes or more should be a sub-chronic toxicity study (90-day).

Conclusion

The Di-tertiary (C9-C12) Alkyl Polysulfides Category underwent the developmental teratology screening test pursuant to OECD Test Guideline 414 (Teratogenicity). This study fulfills the HPV requirements for this SIDS endpoint, and no additional testing is proposed (see Table 16 and IUCLID Documents).

The Subchronic Oral Toxicity – Rodent 90-day Study (OECD 408) with a focus on reproductive endpoints is proposed for di-tertiary nonyl polysulfide, which in combination with the Developmental Toxicity study will fulfill the Reproductive Toxicity endpoint. Current EPA and OECD guidance states that "When a 90-day repeated dose study is available and demonstrates no effect on reproductive organs, in particular the testes, then a developmental study (e.g. OECD Test guidelines 414) can be considered as an adequate test to complete information on reproduction/developmental effect" (USEPA, 1998; OECD, 2002). Reproductive endpoints to be incorporated into the 90-Day Subchronic Toxicity study might include: gonadal weight and size, gonadal histopathology, accessory sex organ weight and size, accessory sex organ gross pathological appearance, accessory sex organ histopathology, spermatogenesis, sperm count and quality assessment, and estrus cyclicity. OECD (2002) has determined that these reproductive endpoints are either already incorporated into the 90-Day Subchronic Guidelines (OECD 407, 408, 409, and 412) or can be included in the study design without significant disruption to study methodology (OECD, 2002).

The Subchronic Oral Toxicity – Rodent 90-day Study was also chosen by the Polysulfides Scientific Research Program in order to meet future anticipated ICCA and REACH testing requirements and to eliminate unnecessary and/or duplicate testing. This is consistent with USEPA's position on chemicals which are being tested in multiple programs (e.g., HPV Challenge Program and the VCCEP program) where EPA states that "sponsors should consider conducting appropriate upper tier test(s) instead of the screening studies (such as OECD 422 or OECD 407 and 415/421 studies) included in the HPV Challenge Program to avoid conducting the lower tier studies unnecessarily" (USEPA, 2000).

2.2 Initial Assessment for Human Health

Data are available for the majority of the human health toxicity endpoints, as provided in Tables 7 through 16 and described above. However, there were insufficient data to fulfill the Reproductive Toxicity endpoint. The 90-day Subchronic Oral Toxicity study in rodents (OECD 408) is proposed.

3 HAZARDS TO THE ENVIRONMENT

3.1 Aquatic Effects

Acute Toxicity Test Results

Acute fish, daphnid, and algal growth inhibition studies were conducted on this Category according to the relevant OECD/EPA guidelines, and no toxicity was observed at the solubility limit.

Table 17. Aquatic Effects - Acute Toxicity Test Results.

Test	di-tertiary nonyl polysulfide	di-tertiary dodecyl pentasulfide
Acute/Prolonged Toxicity to Fish	Not toxic at maximal conc. corresponding to solubility limit (<0.11 mg/L)	ND
Acute Toxicity to Aquatic Invertebrates (*Daphnia*)	ND	No immobilization after reaching solubility limit of TS. Solubility limit was below the range of quantification (0.1 mg/L) and above the detection limit (0.02 mg/L) of the analytical method. 0.03 mg/L < Solubility limit <0.1 mg/L
Acute Toxicity to Aquatic Plants (Algae)	ND	No inhibition of growth at solubility limit (0.08 mg/L)

Source: Atofina, 2003.
ND = No Data Available

Toxicity to Microorganisms

Toxicity to microorganisms was determined for di-tertiary dodecyl pentasulfide. In this study, it was not possible to detect an inhibitory effect of the substance toward *Pseudomonas putida* even when dimethylformamide or ultrasonic dispersions were used. The maximum concentration tested was 10 g/L.

3.2 Terrestrial Effects

No data available

3.3 Other Environmental Effects

3.4 Initial Assessment for the Environment

Adequate data are available for the Di-tertiary (C9-C12) Alkyl Polysulfides Category for the HPV-required SIDS environmental endpoints. No additional testing is proposed for the purposes of the HPV program.

4 RECOMMENDATIONS

The chemical is a candidate for further testing to fulfill SIDS endpoints as follows:

Limited physiochemical data are available for members of the Category and the Polysulfides Scientific Research Program therefore proposes to complete the following testing for di-tertiary nonyl polysulfide:

- Melting Point (OECD Guideline 102, "Melting Point/Melting Range")
- Boiling Point (OECD Guideline 103, "Boiling Point")
- Vapor Pressure (OECD Guideline 104, "Vapour Pressure")
- Partition Coefficient (OECD Guideline 117,"Partition Coefficient (n-octanol/water), High Performance Liquid Chromatography (HPLC) Method")
- Water Solubility (OECD Guideline 105, "Water Solubility")

Data are available for the majority of the human health toxicity endpoints, however; there were insufficient data to fulfill the Reproductive Toxicity endpoint and therefore, testing is proposed. According to the annex VII of the proposal (dated 29.10.2003) for a regulation of the European parliament and of the council concerning the Registration, Evaluation, Authorisation and Restrictions of chemicals (REACH), an additional standard information requirement for substances manufactured or imported in quantities of 100 tonnes or more should be a sub-chronic toxicity study (90-day). In order to meet future ICCA and REACH testing requirements and to eliminate unnecessary and/or duplicate testing, the Polysulfides Scientific Research Program proposes to perform a Sub-chronic Oral Toxicity – Rodent 90-day Study (OECD 408) with a focus on reproductive endpoints. This study, in combination with the existing Developmental Toxicity study, will fulfill the Reproductive Toxicity endpoint. Current EPA and OECD guidance states that "When a 90-day repeated dose study is available and is sufficiently documented with respect to studying effects on the reproductive organs, and a developmental study is available, the requirements for the reproductive toxicity endpoints are satisfied" (USEPA, 1998; OECD 2002). Di-tertiary nonyl polysulfide is recommended for this test because of its lower molecular weight (and is therefore incrementally less hydrophobic) and represents a potentially more bioavailable fraction of the Di-tertiary (C9-C12) Alkyl Polysulfides Category.

5 REFERENCES

Atofina, 2003. IUCLID Data Set, CAS No. 31565-23-8, di(tert-dodecyl) pentasulphide. Atofina, Paris, France.

Commission of the European Communities (EC). 2003. Proposal for a Regulation of the European Parliament and of the Council Concerning the Registration, Evaluation, Authorisation and Restrictions of Chemicals (REACH), COM(2003) 644, Volume II, Brussels, 29 October 2003.

Klimisch, H.J., E. Andreae, and U. Tillmann. 1997. A systematic approach for evaluating the quality of experimental and ecotoxicological data. *Reg. Tox. and Pharm*. 25: 1-5.

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USEPA, Office of Pollution Prevention and Toxics and Syracuse Research Corporation. 2000. EPI Suite v 3.10 (April, 2001).

ANNEX I: DI-TERT NONYL POLYSULFIDE IUCLID DOCUMENTS

See attached IUCLID documents.

ANNEX II: DI-TERT DODECYL PENTASULFIDE IUCLID DOCUMENTS

See attached IUCLID documents.

ANNEX III: DATA QUALITY ASSESSMENT

Available environmental, ecotoxicity, and mammalian toxicity studies were reviewed and assessed for reliability according to standards specified by Klimisch et al., (1997), as recommended by the USEPA (1999a) and the OECD (OECD, 2002). The following reliability classification (Klimisch rating) has been applied to each study assessed:

- *1 = Reliable without Restriction* – Includes studies that comply with USEPA- and/or OECD-accepted testing guidelines and were conducted using Good Laboratory Practices (GLPs) and for which test parameters are complete and well documented;

- *2 = Reliable with Restriction* – Includes studies that were conducted according to national/international testing guidance and are well documented. May include studies that were conducted prior to establishment of testing standards or GLPs but meet the test parameters and data documentation of subsequent guidance; also includes studies with test parameters that are well documented and scientifically valid but vary slightly from current testing guidance. Also included in this category were physical-chemical property data obtained from reference handbooks, as well as environmental endpoint values obtained from an accepted method of estimation (e.g., USEPA's EPIWIN estimation program);

- *3 = Not Reliable* – Includes studies in which there are interferences in either the study design or results that provide scientific uncertainty or in which documentation is insufficient; and,

- *4 = Not Assignable* – This designation is used in this dossier for studies that appear scientifically valid but for which insufficient information is available to adequately judge robustness.

Those studies receiving a Klimisch rating of 1 or 2 are considered adequate to support data assessment needs in this dossier. Those key studies selected for inclusion are considered typical of the endpoint responses observed in other studies of a similar nature and design that were identified during our search of the literature.

I U C L I D

Data Set

Existing Chemical	:	ID: 68425-16-1
CAS No.	:	68425-16-1
EINECS Name	:	Polysulfides, di-tert-nonyl
EC No.	:	270-336-2
Molecular Weight	:	414
Structural Formula	:	C9H19-S-S-S-S-S-C9H19
Molecular Formula	:	C18H38S5
Generic name	:	TPS 37

Producer related part

Company	:	Atofina
Creation date	:	09.07.2001

Substance related part

Company	:	Atofina
Creation date	:	09.07.2001
Status	:	
Memo	:	
Printing date	:	16.04.2004
Revision date	:	
Date of last update	:	16.04.2004
Number of pages	:	28
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS, temporary flag

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	
Name	:	Atofina
Contact person	:	
Date	:	
Street	:	4-8, cours Michelet La Défense 10
Town	:	95091 Paris La Défense Cedex
Country	:	France
Phone	:	+33 1 49 00 80 80
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

01.04.2004

Type	:	
Name	:	ATOFINA Chemicals Inc.
Contact person	:	
Date	:	
Street	:	2000 Market Street
Town	:	PA 19103 Philadelphia
Country	:	United States
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

01.04.2004

Type	:	
Name	:	Chevron Phillips Chemical Company LP
Contact person	:	
Date	:	
Street	:	10001 Six Pines Drive
Town	:	77380 The Woodlands, TX
Country	:	United States
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

16.04.2004

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type :
Substance type : organic
Physical status : liquid
Purity :
Colour :
Odour :

30.07.2003

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

Di-t-nonyl polysulfide

Source : Chevron Phillips Chemical Company LP The Woodlands, TX
08.12.2003

t-Nonyl polysulfide

Source : Chevron Phillips Chemical Company LP The Woodlands, TX
08.12.2003

tertiary-Nonyl polysulfide

Source : Chevron Phillips Chemical Company LP The Woodlands, TX
08.12.2003

TNPS, TPS 37

Source : ELF ATOCHEM ROTTERDAM B.V. VONDELINGENPLAAT/Rt
30.07.2003

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

Remark : Production process : Oxidation of nonyl mercaptan and mineral sulphur.
Two production plant.
Individual protective equipment (gloves, goggles).

Source : ELF ATOCHEM Paris la defense 10
30.07.2003

1.11 ADDITIONAL REMARKS

Remark : Transport : UN Number 3082
ADR/RID : Class 9 ; Item (letter) : 11°c ; Labels : 9 ;
H.I.Nr/ID Nr : 90/3082 ;
IMDG : Class 9 ; UN nr : 3082 ; Packaging group : III ;
Labels : MARINE POLLUTANT
IATA : Class : 9 ; Packaging group : III ; UN Nr(IATA) or
IDNr : 3082 ; Labels : 9.

Source : ELF ATOCHEM Paris la defense 10
30.07.2003

1.12 LAST LITERATURE SEARCH

Type of search : Internal and External
Chapters covered : 3, 4, 5
Date of search : 14.01.2004

Source : Atofina, Paris La Défense, France (JFR)
14.01.2004

Type of search : Internal and External
Chapters covered : 2
Date of search : 14.01.2004

Source : Atofina, Paris La Défense, France (JFR)
14.01.2004

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= 96.7 °C
Sublimation	:	
Method	:	other: calculated using EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di-tert nonyl polysulfide (CAS Number 68425-16-1)
Method	:	MPBPWIN (v 1.40) Selected Melting Point (Mean Value).
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

04.03.2004 (1)

Value	:	= -29 °C
Sublimation	:	
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	other TS
Test substance	:	TPS 37, DITERTIONONYL PENTASULFIDE, CAS: 68425-16-1
Source	:	Atofina, Paris-La Défense, France.
Reliability	:	(4) not assignable

08.01.2004 (2)

2.2 BOILING POINT

Value	:	= 350.6 °C at
Decomposition	:	
Method	:	other: calculated using EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di-tert nonyl polysulfide (CAS Number 68425-16-1)
Method	:	MPBPWIN (v 1.40) Boiling Point (Adapted Stein and Brown Method).
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

04.03.2004 (1)

Value	:	> 200 °C at
Decomposition	:	
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	other TS
Test substance	:	TPS 37, DITERTIONONYL PEBTASULFIDE, CAS no.68425-16-1
Source	:	Atofina, Paris-La Défense, France
Reliability	:	(4) not assignable

08.01.2004 (2)

2.3 DENSITY

Type	:	density
Value	:	= 1.024 g/cm³ at 20 °C
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	other TS
Source	:	Atofina, Paris-La Défense, France
Test substance	:	TPS 37, DITERTIONONYL PETASULFIDE, CAS no.68425-16-1
Reliability	:	(4) not assignable

08.01.2004 (2)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	= .0000343 hPa at 25 °C
Decomposition	:	
Method	:	other (calculated): EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di-tert nonyl polysulfide (CAS Number 68425-16-1)
Method	:	EPIWIN Selected Vapor Pressure (Modified Grain Method). Vapor Pressure Estimations (25 deg C) using BP: 350.62 deg C (estimated) and MP: 96.7 deg C (estimated).
Remark	:	3.43E-5 hPa = 2.57E-5 mmHg.
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

04.03.2004 (1)

Value	:	< .03 hPa at 20 °C
Decomposition	:	
Method	:	other (calculated): no data
Year	:	
GLP	:	no data
Test substance	:	other TS
Test substance	:	TPS 37, DITERTIONONYL PENTASULFIDE, CAS no.68425-16-1
Source	:	Atofina, Paris-La Défense, France
Reliability	:	(4) not assignable

08.01.2004 (2)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	
Log pow	:	= 9.14 at °C
pH value	:	

Method	:	other (calculated): EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Method	:	WSKOW v 1.40 -- estimated Log Kow.
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Test substance	:	di-tert nonyl polysulfide (CAS Number 68425-16-1)
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

04.03.2004 (1)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	not soluble
Stable	:	
Deg. product	:	
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	other TS
Test substance	:	TPS 37, DITERTIONONYL PENTASULFIDE, CAS no.68425-16-1
Source	:	Atofina, Paris-La Défense, France
Reliability	:	(4) not assignable

08.01.2004 (2)

Solubility in	:	
Value	:	= .0001 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated using EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di-tert nonyl polysulfide (CAS Number 68425-16-1)
Method	:	Water Solubility calculated from Kow (WSKOW v 1.40).
Result	:	Calculated Water Solubility = 9.612E-5 mg/L
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

15.12.2003 (1)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value	:	= 100 °C
Type	:	closed cup
Method	:	other: ASTM D93
Year	:	
GLP	:	no data
Test substance	:	other TS
Source	:	Atofina, Paris-La Défense, France
Test substance	:	TPS 37, DITERTIONONYL PENTASULFIDE, CAS no.68425-16-1
Reliability	:	(4) not assignable

08.01.2004 (2)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

Value	:	= 183.5 - mPa s (dynamic) at 20 °C
Result	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS
Source	:	Atofina, Paris-La Défense, France
Test substance	:	TPS 37, DITERTIONONYL PENTASULFIDE, CAS no.68425-16-1
Reliability	:	(4) not assignable

08.01.2004 (2)

Value	:	= 24 - 34 mPa s (dynamic) at 50 °C
Result	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS
Source	:	Atofina, Paris La-Défense, France.
Test substance	:	TPS 37, DITERTIONONYL PEBTASULFIDE, CAS no.68425-16-1
Reliability	:	(4) not assignable

08.01.2004 (2)

Value	:	= 4 - mPa s (dynamic) at 100 °C
Result	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS

Source	:	Atofina, Paris-La Défense, France
Test substance	:	TPS 37, DITERTIONONYL PEBTASULFIDE, CAS no.68425-16-1
Reliability	:	(4) not assignable

08.01.2004 (2)

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	**other**
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
Deg. product	:	
Method	:	other (calculated): EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di-tert nonyl polysulfide (CAS Number 68425-16-1)
Method	:	Calculated using EPIWIN v 3.10, AOP Program v 1.90.
Result	:	Overall OH Rate Constant = 473.0059 E-12 cm3/molecule-sec Half-Life = 0.023 Days (12-hr day; 1.5E6 OH/cm3) Half-Life = 16.281 Min
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

09.12.2003 (1)

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	**fugacity model level III**
Media	:	other: air-water-soil-sediment
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: EPIWIN v 3.10
Year	:	2003
Test substance	:	di-tert nonyl polysulfide (CAS Number 68425-16-1)
Method	:	Used EPIWIN v 3.10. The following physical properties were used as the model input parameters: Chem Name: Di-tertiary-nonyl polysulfide Molecular Wt: 350.68 Henry's LC: 0.174 atm-m3/mole (Henrywin program) Vapor Press: 2.57E-5 mm Hg (Mpbpwin program)

Liquid VP: 0.000132 mm Hg (super-cooled)
Melting Pt: 96.7 deg C (Mpbpwin program)
Log Kow: 9.14 (Kowwin program)
Soil Koc: 5.66E+8 (calc by model)

Result : Results are provided in the following format:
Compartment / 100% to Air / 100% to Water / 100% to Soil / Equally to Each Compartment

Air / 75.0% / 3.95E-6% / 4.06E-6% / 0.00474%
Water / 0.0745% / 1.87% / 0.0021% / 1.28%
Soil / 21.0% / 5.13E-7% / 99.9% / 31.6%
Sediment / 3.91% / 98.1% / 0.11% / 67.1%

Air: half life = 0.5426 hr; emissions = 1000 kg/hr
Water: half life = 3600 hr; emissions = 1000 kg/hr
Soil: half life = 3600 hr; emissions = 1000 kg/hr
Sediment: half life = 1.44E+4 hr; emissions = 0 kg/hr

Persistence when distributed equally to each compartment = 5.47E+3 hr (Emissions [kg/hr] = 1000 to air, 1000 to water, 1000 to soil, and 0 to sediment).

Source : EPI Suite v 3.10.
Chevron Phillips Chemical Company LP The Woodlands, TX

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
10.12.2003 (1)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : **aerobic**
Inoculum : other: River water
Concentration : 800 mg/l related to Test substance
related to
Contact time : 28 day(s)
Degradation : < 0 (±) % after 28 day(s)
Result : under test conditions no biodegradation observed
Kinetic of testsubst. : 7 day(s) < 0 %
14 day(s) < 0 %
22 day(s) < 0 %
28 day(s) < 0 %
%
Control substance : Benzoic acid, sodium salt
Kinetic : 7 day(s) = 35.9 %
28 day(s) = 52.4 %
Deg. product : not measured
Method : Directive 84/449/EEC, C.6 "Biotic degradation - closed bottle test"
Year :
GLP : no data
Test substance :

Test substance : Test compound: TPS 37
Chemical name: di-t-nonyl polysulfide
CAS no.: 68425-16-1

Origine: Atochem
Batch: 6253
Total sulfur: no data

Test condition : INOCULUM/TEST ORGANISM
- Type of sludge: River water.
- Sampling site: Levallois
- Preparation of inoculum: Water was deducted from the river, decantated and filtred on a 0.22µm filter.The filter was rinsed with water and introduced for sowing flasks.
- Pretreatment:
- Initial cell concentration: 50 µl/l.

TEST SYSTEM
- Culturing apparatus: 300ml Erlenmeyers flasks.
- Number of culture flasks per concentration: 10.
- Aeration device: The solution was saturated with compressed air for 6 hours.
- Measuring equipment:Closed bottles.
- Closed vessels used: Yes.

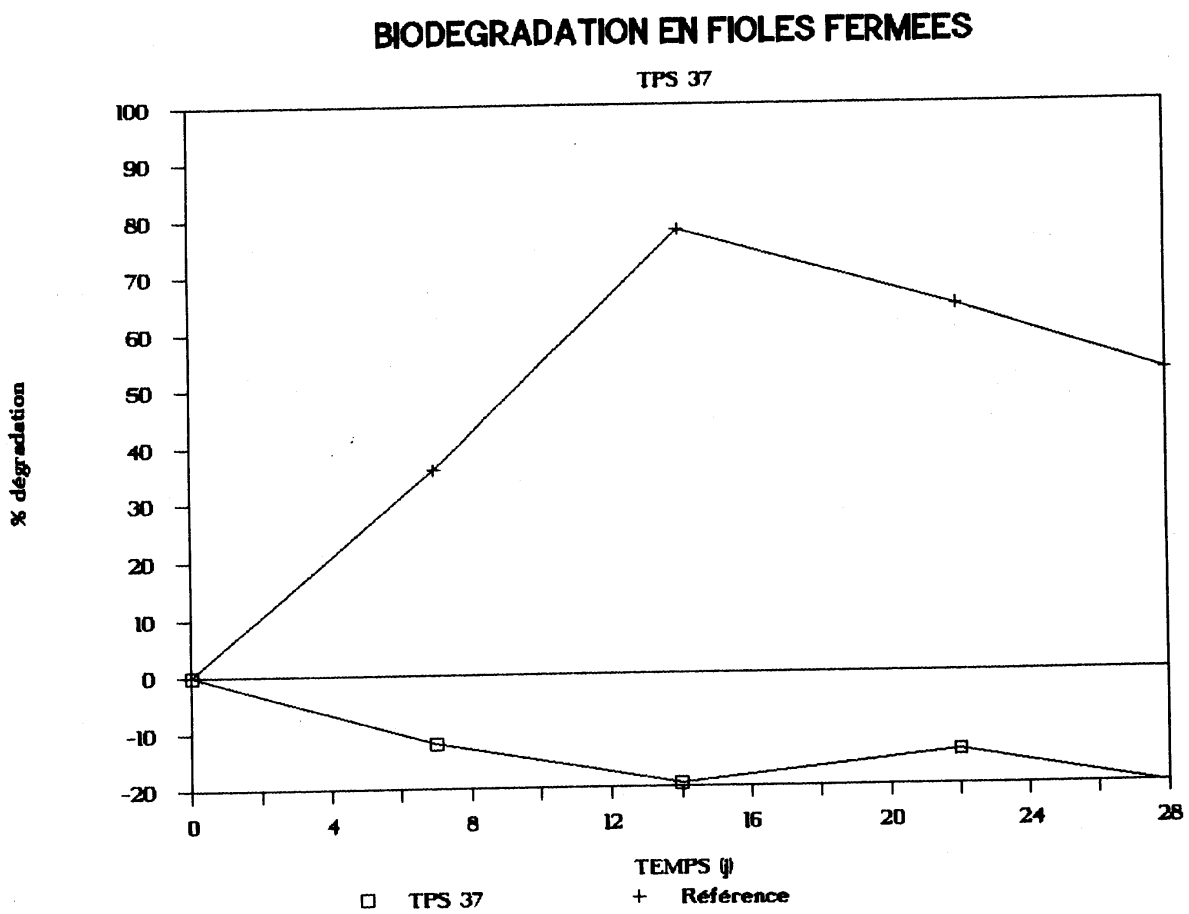
INITIAL TEST SUBSTANCE CONCENTRATION: 800 mg/l.
METHOD OF PREPARATION OF TEST SOLUTION:The substance was insoluble so it was introduced with acetone solvent which was evaporated before the test.
DURATION OF THE TEST: 28 days.
ANALYTICAL PARAMETER: The consumption of oxygen in the solution.The bacterial activity is evaluated by the consumption of dissolved O2, and the degradation follows from the difference between its consumption in flasks containing test substance and check flasks.
SAMPLING: 7, 14, 22, 28 days.
TEST CONDITIONS
- Composition of medium: For one litre of saturated water(with O2):

1- 1ml of solution a: KH_2PO_4 8.50g
K_2HPO_4 21.75g
Na_2HPO_4 33.40g
H_2O 1 litre.
2- 1ml of solution b: NH_4Cl 0.5g
H_2O 1 litre.
3- 1ml of solution c: $CaCl_2$ 27.5g
H_2O 1 litre.
4- 1ml of solution d: $MgSO_4,7H_2O$ 22.50 g
H_2O 1 litre.
5- 1ml of solution e: $FeCl_3$ 0.25g
E.D.T.A 0.40g
H_2O 1 litre.
6- water q.s.p 1000 ml.

- Additional substrate: No.
- Test temperature: 21+/-1°C.

INTERMEDIATES / DEGRADATION PRODUCTS: Not identified.
NITRATE/NITRITE MEASUREMENT: No.
CONTROLS:
REFERENCE SUBSTANCE: Benzoic acid,sodium salt.

Attached document : Courbe.bmp
Resultats.bmp



BIODEGRADATION EN FIOLES FERMEES

SUBSTANCE D'ESSAI: TPS 37
SUBSTANCE DE REFERENCE: BENZOATE DE SODIUM

ESSAI	FIOLE	TEMPS D'INCUBATION ,jours				
		0	7	14	22	28
		concentration oxygène (mg/l)				
BLANC	1	8,3	7,3	6,9	7,1	6,8
	2	8,4	7,3	6,9	7,0	6,6
	moyenne	8,35	7,30	6,90	7,05	6,70
ESSAI	1	8,1	7,6	7,5	7,5	7,5
	2	8,0	7,7	7,8	7,5	7,5
	moyenne	8,05	7,65	7,65	7,50	7,50
REFERENCE	1	8,3	6,8	4,4	4,8	5,0
	2	8,2	5,2	4,0	4,8	4,7
	moyenne	8,25	6,00	4,20	4,80	4,85

	Pourcentage de dégradation				
jours	0	7	14	22	28
ESSAI	0,0	-12,0	-19,4	-13,8	-20,3
REFERENCE	0,0	35,9	77,8	64,4	52,4

DThO (mg O2 / l)	
TPS 37	2,71
PhCOONa	1,67

Remark : Study Peer Reviewed.

Source	:	ATOFINA, PARIS-LA-DEFENSE, FRANCE.
Reliability	:	(1) valid without restriction
Flag	:	Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

16.04.2004 (3)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

BCF	:	75.66
Elimination	:	
Method	:	other: calculated using EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Method	:	Calculated using BCF Program (v 2.14).
Remark	:	Estimated Log BCF = 1.879 Estimated Koc = 2.797E+5 (using PCKOCWIN v 1.66)
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions

10.12.2003 (1)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	**static**
Species	:	Brachydanio rerio (Fish, fresh water)
Exposure period	:	96 hour(s)
Unit	:	mg/l
Limit test	:	yes
Analytical monitoring	:	yes
Method	:	Directive 92/69/EEC, C.1
Year	:	1992
GLP	:	yes
Test substance	:	

Test substance :

Test compound: TPS 37
Chemical name: di-t-nonyl polysulfide
CAS no.: 68425-16-1
Origine: Elf Atochem
Batch: no data
Total sulfur: 35.7% w/w

Test condition :

TEST ORGANISMS
- Strain: Brachydanio rerio.
- Supplier: Fish farming HB development, St Fargeux, FRANCE.
- Length: The animals were ranging from 3.1 to 3.3 cm.
- Acclimatisation: Animals were acclimated for 70 days in water (same quality, same temperature, same light... used in the test).

STOCK AND TEST SOLUTION AND THEIR PREPARATION
- Procedures: The test substance was dissolved in aqueous solution at 100 mg/l, agitated mechanically for 65 hours at 23°C.The substance not dissolved was filtered on Millipore GV 0.22µm.

DILUTION WATER:
According to EEC method C.1 92/69.
- 294 mg/l CaCl2, 2H2O
- 123.3 mg/l MgSO4, 7H2O
- 63.0 mg/l NaHCO3
- 5.5 mg/l KCl

TEST SYSTEM
- Nominal concentrations: 0.1 to 100 % vol.
- Number of replicates, fish per replicate: 5 fish per concentration
- Test temperature: 23.5+-1°C.
- Controled lighting : darkness 12/hours/24h)

The test was performed in 5 l glass crystallizing dishes closed with Altuglas plates.
2 vessels and 10 fishes were used per concentration.

TEST PARAMETER: Mortality or visible abnormalities.
MONITORING OF TEST SUBSTANCE CONCENTRATION: HPLC/MS.

Limit Test :
Saturated solution at 100 mg/l substance

- pH

Th	0	24	48	72	96
Saturated solution	8.60	7.80	7.81	7.91	7.76
Blank	7.86	7.83	7.80	7.82	7.79

- O2
Saturated 8.6 7.4 7.7 7.8 7.4
solution
Blank 8.5 7.8 7.8 7.6 7.7

Result : MORTALITY(%)

	24h	48h	72h	96h
Saturated solution	0	0	0	0
Blank	0	0	0	0

At the solubility limit of the substance in the test medium, no death of fishes was recorded at 96 hours.Thus, The substance was not toxic at the maximal concentration corresponding to the solubility limit in the test medium,
< 0.11 mg/l.

The study was performed in compliance with the following quality criteria : mortality in the control did not exceed 10% at the end of the test;concentration of dissolved oxygen in the test vessels remained above 60% of the air saturation value at the end of the test;pH did not vary by more than 1 unit.
Since it was not possible to determine the concentration of the substance at the limit of solubility (<0.11 mg/l), the validity criteria related to the test substance stability has not be checked.

Source : Atofina, Paris la Défense, France.
Reliability : (1) valid without restriction
Flag : Directive 67/548/EEC, Critical study for SIDS endpoint
16.04.2004 (4)

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	**LD50**
Value	:	= 17781 - 21495 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	40
Vehicle	:	other: none
Doses	:	16000, 18000, 22000 and 24000 mg/kg
Method	:	other: comparable to OECD Guide-line 401
Year	:	
GLP	:	no
Test substance	:	

Test substance :

Test compound: TPS 37
Chemical name: di-t-nonyl polysulfide
CAS no.: 68425-16-1
Origine: Elf Aquitaine
Batch: no data
Total sulfur: no data

Test condition :

TEST ORGANISMS:
- Source: IFFA-CREDO
- Age: no data
- Weight at study initiation: 140-170 g
- Controls: no

ADMINISTRATION:
- Volume administered: 16 to 24 ml/kg of the undiluted test compound
- Post dose observation period: no

EXAMINATIONS: All animals were observed for mortality and signs of toxicity at 1, 2 and 6 hours post-dose and once daily thereafter for 14 consecutive days.
Individual body weights were recorded prior to treatment, on days 1, 2, 4, 7 and at termination.

STATISTICAL TEST: Mortality data were analyzed by the Litchfield and Wilcoxon's method

Result :

MORTALITY:

Dose mg/kg	Male	Female	Total
16000	2/5	0/5	2/10
18000	2/5	1/5	3/10
22000	1/5	5/5	6/10
24000	4/5	4/5	8/10

CLINICAL SIGNS:
- 16000 and 18000 mg/kg:
1 hour after treatment: lower spontaneous activity, apathy, prostration, piloerection, staggering step, slight closing of the palpebral slit .
6 hour after treatment: same symptoms.

Day 1 and 2: piloerection
Dqay 3: the surviving animals were normal.

-22000 et 24000 mg/kg:
Severe reduction of the spontaneous activity, apathy, prostration, staggering step. Loss of the reversal reflex in a female (24000 mg/kg).
6-24 hours after treatment: same clinical signs and diarrhea.
Day 2 : Piloerection in the surviving animals.
Day 3:
- 22000 mg/kg, recovery in the surviving animals.
- 24000 mg/kg distended abdomen.

Conclusion : The oral LD50 of TPS37 was 19550 (17781-21495) mg/kg.
Source : Atofina, Paris-la-Défense, France.
Reliability : (2) valid with restrictions
Flag : Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

26.02.2004 (5)

5.1.2 ACUTE INHALATION TOXICITY

Type : **LC50**
Value : > 15.5 mg/l
Species : rat
Strain : Sprague-Dawley
Sex : male/female
Number of animals : 10
Vehicle : other: none
Doses : 15.5 mg/l
Exposure time : 4 hour(s)
Method : other: comparable to OECD Guide-line 403
Year :
GLP : no
Test substance :

Test substance : Test compound: TPS 37
Chemical name: di-t-nonyl polysulfide
CAS no.: 68425-16-1
Origine: Elf Aquitaine
Batch: no data
Total sulfur: no data

Test condition : TEST ORGANISMS:
- Source: IFFA-CREDO
- Age: no data
- Weight at study initiation: 150-200 g
- Number of animals: 5 males + 5 females
- Controls: no

ADMINISTRATION:
- Type of exposure: whole body
- Atmosphere generation: controlled fluid feed from a disposable plastic syringe driven by a syringe pump
- Concentration: nominal

EXAMINATIONS:
Duration of observation: 14 days
- Clinical signs: continuously during the exposure period, then daily until final sacrifice.
- Mortality: recorded once daily until the completion of the study.
- Body weight: measured on days 1, 3, 7 and 14.
- Necropsy: macroscopic examination of the main organs.

Result	:	CLINICAL SIGNS: . During exposure: From the very start of the exposure a very dense white fog settles in the chamber and limit the observation of the animals which remain huddled during the exposure. Only a reduction in the reaction to the noises from 45 min up to the absence of reaction can be highlighted. . After exposure: At the removal from the chamber the animals have wet fur and seek to flee. They present a slight irritation of the muzzle but recover a normal spontaneous activity after 15 mn. J 1: Closing of the palpebral slit, eyes cyanosed, polypnea and bronchial obstruction. J 2: one male died. J 4: all normal. NECROPSY: clear lungs
Conclusion	:	The inhalation exposur for 4 hours of 10 rats to a nominal concentration of 15.5 g/m3 TPS37 induced a mortality of 10%.
Source	:	Atofina, Paris-la-Défense, France.
Reliability	:	(2) valid with restrictions
Flag	:	Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

26.02.2004 (6)

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

Type	:	**LD50**
Value	:	= 3350 - 4375 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	30
Vehicle	:	other: none
Doses	:	3500, 4500 and 6000 mg/kg
Route of admin.	:	i.p.
Exposure time	:	
Method	:	other
Year	:	
GLP	:	no
Test substance	:	
Test substance	:	Test compound: TPS 37 Chemical name: di-t-nonyl polysulfide CAS no.: 68425-16-1 Origine: Elf Aquitaine Batch: no data Total sulfur: no data
Result	:	MORTALITY:

Dose (mg/kg)	Males	Females
3500	0/5	4/5
4500	2/5	5/5
6000	5/5	5/5

LD50: 3828 (3350-4375) mg/kg

CLINICAL SIGNS:
- 3 500 mg/kg:
1 hour after treatment: reduced spontaneous Activity, apathy, prostration, piloerection, slight closing of the palpebral slit
6 hours after treatment: same as above
D 2: Piloerection
D 3: Piloerection and eyes cyanosed in one female. Other survivors look normal

- 4 500 mg/kg:
Just after treatment: low spontaneous Activity, apathy, prostration, piloerection, closing of the palpebral slit
6 hours after treatment: moribund animals
D 1: Recovery of survivors
- 6 000 mg/kg: same as above, but more prononced, loss of the turning over reflexe.

Source : Atofina, Paris-la-Défense, France.
Reliability : (2) valid with restrictions
26.02.2004 (7)

5.2.1 SKIN IRRITATION

Species : rabbit
Concentration : undiluted
Exposure : Occlusive
Exposure time : 24 hour(s)
Number of animals : 6
Vehicle :
PDII : 1.88
Result : slightly irritating
Classification : irritating
Method : other: JO RF 21/4/71, 5/6/73
Year : 1973
GLP : no
Test substance :

Test substance : Test compound: TPS 37
Chemical name: di-t-nonyl polysulfide
CAS no.: 68425-16-1
Origine: Elf Aquitaine
Batch: no data
Total sulfur: no data
Source : Atofina, Paris-la-Défense, France.
Reliability : (2) valid with restrictions
Flag : Material Safety Dataset, Directive 67/548/EEC
26.02.2004 (8)

5.2.2 EYE IRRITATION

Species : rabbit
Concentration : undiluted
Dose : .1 ml
Exposure time : 24 hour(s)
Comment : not rinsed
Number of animals : 6
Vehicle :
Result : slightly irritating

Classification	:	not irritating
Method	:	other: JO RF 21/04/71 & 05/06/73
Year	:	1973
GLP	:	no
Test substance	:	
Test substance	:	Test compound: TPS 37 Chemical name: di-t-nonyl polysulfide CAS no.: 68425-16-1 Origine: Elf Aquitaine Batch: no data Total sulfur: no data
Source	:	Atofina, Paris-la-Défense, France.
Reliability	:	(2) valid with restrictions
Flag	:	Material Safety Dataset, Directive 67/548/EEC

26.02.2004 (8)

5.3 SENSITIZATION

Type	:	**Guinea pig maximization test**
Species	:	guinea pig
Concentration	:	1st: Induction 25 % intracutaneous 2nd: Induction 50 % occlusive epicutaneous 3rd: Challenge 1 % occlusive epicutaneous
Number of animals	:	30
Vehicle	:	
Result	:	not sensitizing
Classification	:	not sensitizing
Method	:	Directive 96/54/EC, B.6
Year	:	1996
GLP	:	yes
Test substance	:	other TS
Test substance	:	Test compound: TPS 37 LS Origine: Atofina SA Batch: 30-01-GF Total sulfur: 36.75% (w/w) Mercaptans: 1 ppm
Method	:	Thirty guinea pigs were allocated to two groups: a control group of five males and five females and a treated group of ten males and ten females. On day 1, three pairs of intradermal injections were performed in the interscapular region of all animals: · Freund's complete adjuvant (FCA) diluted at 50% (v/v) with 0.9% NaCl (both groups), · test item at the chosen concentration in the chosen vehicle (treated group) or vehicle alone (control group), · test item at the chosen concentration in a mixture FCA/0.9% NaCl (50/50, v/v) (treated group) or vehicle at the concentration of 50% (w/v) in a mixture FCA/0.9% NaCl (50/50, v/v) (control group). On day 8, the test item (treated group) or the vehicle (control group) was applied topically to the same test site, which was then covered by an occlusive dressing for 48 hours. On day 22, all animals of both groups were challenged by a cutaneous application of the test item to the right flank. The left flank served as control and received the vehicle only. The test item and vehicle were maintained under an occlusive dressing for 24 hours. Skin reactions were evaluated approximately 24 and 48 hours after

removal of the dressing.

Test item concentrations were as follows:

Induction (treated group)
· intradermal injections (day 1): TPS 37 LS at the concentration of 25% (w/w) in corn oil,
· topical application (day 8): TPS 37 LS at the concentration of 50% (w/w) in acetone.

Challenge (all groups)
· topical application (day 22): TPS 37 LS at the concentration of 1% (w/w) in acetone.

At the end of the study, animals were killed without examination of internal organs.
No skin samples were taken from the challenge application sites.

Result : No clinical signs and no deaths related to treatment were noted during the study.

No cutaneous reactions were observed after the challenge application.

Conclusion : According to the maximization method of Magnusson and Kligman, the test item TPS 37 LS (batch No. 30-01-GF) at the concentration of 1% does not induce delayed contact hypersensitivity in guinea pigs

Source : Atofina, Paris-la-Défense, France.
Reliability : (1) valid without restriction
Flag : Material Safety Dataset, Directive 67/548/EEC
26.02.2004 (9)

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

Type : **Salmonella typhimurium reverse mutation assay**
System of testing : Strains: TA 98, TA 100, TA 1535, TA 1537, TA 102
Test concentration : Experiment 1: 8, 40, 200, 1000 and 5000 µg/plate
Experiment 2: 4.883, 19531, 78.125, 312.5, 1250 and 5000 µg/plate
Cycotoxic concentr. : >= 1250 µg/plate
Metabolic activation : with and without
Result : negative
Method : Directive 84/449/EEC, B.14
Year : 1993
GLP : yes
Test substance :

Test substance : Test compound: TPS 37
Chemical name: di-t-nonyl polysulfide
CAS no.: 68425-16-1
Source: Elf Aquitaine Production
Batch: 47978
Sulfur content: 36.9%.

Test condition : SYSTEM OF TESTING
- 2 independent trials; in the 1st and 2nd trial without metabolic activation system (MA) the direct plate incorporation method was used; this method also used in the 1st trial with MA, in the 2nd trial with MA the preincubation method (1 h, 37°C). 3 plates per concentration
- Metabolic activation system (MA): S9 fraction from liver homogenates of rats induced with 500 mg/kg Aroclor 1254

- solvent: dimethylformamide
- Controls: . solvent control (with and without MA)
. Positives controls:
- Without S9
TA98: 2-nitrofluorene 5.0 µg/plate
TA100 and TA1535: Sodium azide 2.0 µg/plate
TA1537: 9-aminoacridine 50 µg/plate
TA102: glutaraldehyde 25 µg/plate
- With S9
TA98, TA100 and TA1535: 2-aminoanthracene 5.0 µg/plate
. sterility control checked during the test.
- Concentrations:
Experiment 1: 8, 40, 200, 1000 and 5000 µg/plate
Experiment 2: 4.883, 19531, 78.125, 312.5, 1250 and 5000 µg/plate
- Cytotoxicity: A preliminary toxicity test was performed to define the concentrations to be used for the mutagenicity study. TA100 exposed to 8-5000 µg/plate with and without MA

CRITERIA FOR EVALUATION
- negative and positive controls within the range of historical controls.
- positive: reproducible and significant dose related increase in revertants and/or reproducible doubling in the number of revertants compared with negative controls for one dose.

Result : Evidence of toxicity was observed at >=1250 µg/plate in only a few test strains. Precipitation of test agent was observed on all plates treated at concentrations >= 1000 µg/plate.

The mean numbers of revertant colonies on negative control plates all fell within acceptable ranges, and were significantly elevated by positive control treatments.

No TPS 37 treatment of any of the test strains produced an increase in revertant numbers sufficient to be considered as indicative of mutagenic activity.

Conclusion : TPS 37 did not induce mutation in five strains of Salmonella typhimurium (TA98, TA100, TA1535, TA1537 and TA102), when tested under the conditions employed for this study, which included treatments up to 5000 µg/plate, both in the absence and in the presence of a rat liver metabolic activation system (S-9).

Source : Atofina, Paris-la-Défense, France.
Reliability : (1) valid without restriction
Flag : Material Safety Dataset, Critical study for SIDS endpoint
26.02.2004 (10)

Type : **Chromosomal aberration test**
System of testing : Human Lymphocytes
Test concentration : 122.5, 175, 250 µg/ml
Cycotoxic concentr. : see freetext ME
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 473
Year : 1996
GLP : yes
Test substance :

Test substance : Test compound: TPS 37
Chemical name: di-t-nonyl polysulfide
CAS no.: 68425-16-1
Source: Elf Aquitaine Production
Batch: 47978
Sulfur content: 36.9%.

Method : TPS 37 was tested in an in vitro cytogenetics assay using duplicate human lymphocyte cultures from female donors in two independent experiments. The test article was dissolved in dimethyl formamide (used as vehicle control) and the highest dose level used, 250 µg/mL, was in excess of the solubility limit in culture medium.

In Experiment 1, treatment in the absence and presence of S-9 (rat liver post-mitochondrial fraction from Aroclor 1254 induced animals) was for 3 hours only followed by a 17 hour recovery period prior to harvest (3+17). The test article dose levels for chromosome analysis were selected by evaluating the effect of TPS 37 on mitotic index.
Chromosome aberrations were analysed at three consecutive dose levels (see below).
The highest concentration chosen for analysis, 250 µg/mL, induced no mitotic inhibition (reduction in mitotic index) in either the absence or presence of S-9.

S-9	Treatment+ recovery (hours)	Concentration (µg/ml)	Positive control
-	3+17	0, 122.5, 175, 250	NQO,2.5.µg/mL
+	3+17	0, 122.5, 175, 250	CPA, 25 µg/mL

In Experiment 2, treatment in the absence of S-9 was continuous for 20 hours. Treatment in the presence of S-9 (using S-9 prepared from animals induced with phenobarbitone and beta-naphthoflavone) was for 3 hours only followed by a 17 hour recovery period prior to harvest (3+17). Chromosome aberrations were analysed at three consecutive dose levels (see below). The highest concentration chosen for analysis was 250 µg/mL, which induced approximately 45 % and 11 % mitotic inhibition respectively.

S-9	Treatment+ recovery (hours)	Concentration (µg/ml)	Positive control
-	20+0	0, 122.5, 175 250	NQO, 2.5 µg/mL
+	3+17	0, 122.5, 175, 250	CPA, 30 µg/ml

Appropriate negative (solvent and untreated) control cultures were included in test system in both experiments under each treatment condition. The proportion of cell with structural aberrations in solvent cultures fell within historical solvent control ranges. 4-Nitroquinoline 1-oxide and cyclophosphamide were employed as positive control chemicals in the absence and presence of liver S-9 respectively. Cells receiving these were sampled in each experiment, 20 hours after the start of treatment; both compounds induced statistically significant increases in the proportion of cells with structural aberrations.

Result : Cultures treated with TPS 37 in the absence and presence of S-9 exhibited frequences of cells with structural aberrations (excluding gaps) which were similar to levels seen in concurrent negative controls. One culture treated with 122.5 µg/ml TPS 37 for 20 ours in the absence of S-9 exhibited frequencies of cells with structural aberrations which exceeded the historical negative control (normal) range. Insofar as the replicate culture at this dose exhibited frequencies within the normal range, the effect was considered to be of no biological relevance. All other test article treated cultures exhibited frequencies of cells with structural aberrations which fell within the normal range.

Conclusion : TPS 37 did not induce chromosome aberrations in cultured human peripheral blood lymphocytes when tested in excess of its limit of solubility in bo the absence and presence of S-9.

Source : Atofina, Paris-la-Défense, France.

Reliability : (1) valid without restriction

Flag : Material Safety Dataset, Critical study for SIDS endpoint
26.02.2004 (11)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

(1) United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation, 2000. EPI Suite v 3.10 (April, 2001).

(2) ATOFINA. Material safety data sheet. TPS37, DITERTIONONYL PENTASULFIDE, CAS: 68425-16-1, 17/01/2003.

(3) ATOCHEM. TPS 37, EVALUATION EN MILIEU AQUEUX DE LA BIODEGRADATION AEROBIE "ULTIME", ESSAI EN FIOLE FERMEE.CENTRE D'APPLICATION DE LEVALLOIS, RAPPORT n° 23737 LE 08/12/89.

(4) ELF ATOCHEM S.A., CAL, 2002.TPS 37. Toxicité aiguë vis-à-vis des poissons.Report N° 509/99//A.

(5) Elf Aquitaine, Ditertiononyl polysulfure-TPS 37, Essais de toxicité aiguë par voie orale et intrapéritonéale chez le rat. IFREB, study no. 911256, novembre 29, 1979.

(6) Elf Aquitaine, Ditertiononyl polysulfure-TPS 37, Essais de toxicité aïgue par voie repiratoire chez le rat. IFREB, study no. 911211, novembre 15, 1979.

(7) Elf Aquitaine, Ditertiononyl polysulfure-TPS 37, Essais de toxicité aïgue par voie orale et intrapéritonéale chez le rat. IFREB, study no. 911256, novembre 29, 1979.

(8) Elf Aquitaine Production, Ditertiononyl polysulfure (TPS 37), Tests de tolérance locale chez le lapin. IFREB, étude no. 911317, 9 novembre 1979.

(9) Atofina (2002) TPS 37 LS, SKIN SENSITIZATION TEST IN GUINEA PIGS (Maximization method of Magnusson and Kligman). CIT report no. 23043 TSG.

(10) Elf Aquitaine, TPS 37, Reverse mutation in five Histidine-requiring strains of Salmonella typhimurium. Covance Labatories Limited, study no. 154/35-D5140, may 1998.

(11) Elf Aquitaine, TPS 37, Induction of Chromosome Aberrations in Cultured Human Peripheral Blood Lymphocytes. Covance Labatories Limited, study no. 154/36-D5140, july 1998.

I U C L I D

Data Set

Existing Chemical	:	ID: 31565-23-8
CAS No.	:	31565-23-8
EINECS Name	:	di(tert-dodecyl) pentasulphide
Product name	:	TPS 32
EC No.	:	250-702-8
Molecular Formula	:	C24H50S5

Producer related part

Company	:	Atofina
Creation date	:	09.07.2001

Substance related part

Company	:	Atofina
Creation date	:	09.07.2001
Status	:	
Memo	:	chapters 3, 4 and 5 validated
Printing date	:	16.04.2004
Revision date	:	
Date of last update	:	16.04.2004
Number of pages	:	39
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS, temporary flag

1.0.1 APPLICANT AND COMPANY INFORMATION

Type :
Name : Atofina
Contact person :
Date :
Street : 4-8, cours Michelet La Défense 10
Town : 95091 Paris La Défense Cedex
Country : France
Phone :
Telefax :
Telex :
Cedex :
Email :
Homepage :

01.04.2004

Type :
Name : ATOFINA Chemicals Inc.
Contact person :
Date :
Street : 2000 Market Street
Town : PA 19103 Philadelphia
Country : United States
Phone :
Telefax :
Telex :
Cedex :
Email :
Homepage :

01.04.2004

Type :
Name : Chevron Phillips Chemical Company LP
Contact person :
Date :
Street : 10001 Six Pines Drive
Town : 77380 The Woodlands, TX
Country : United States
Phone :
Telefax :
Telex :
Cedex :
Email :
Homepage :

Source : Chevron Phillips Chemical Company LP The Woodlands, TX
04.03.2004

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid
Purity	:	
Colour	:	
Odour	:	

Source : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
11.02.2000

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

TPS 32 ;

Source : Elf Aquitaine Lacq
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

25.05.1994

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

Labelling	:	provisionally by manufacturer/importer
Specific limits	:	
Nota	:	, ,
R-Phrases	:	(53) May cause long-term adverse effects in the aquatic environment
S-Phrases	:	(61) Avoid release to the environment. Refer to special instructions/Safety data sets

04.03.2003

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

Type of limit : other: No occupational exposure limit available
Limit value :

Source : Atofina, Paris-la-Défense, France.
04.03.2003

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

Remark : Reaction of tert-Dodecyl mercaptan with sulfur (element) in presence of a catalyst.
H2S is eliminated by stripping.
Wastes to incinerators.
Hydrogen sulfide detectors.

Source : Elf Aquitaine Lacq
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
06.06.1994

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

Type of search : Internal and External
Chapters covered : 3, 4, 5
Date of search : 04.03.2003

Source : Atofina, Paris-la-Défense, France.
04.03.2003

Type of search : Internal and External
Chapters covered : 2
Date of search : 14.01.2004

Source : Atofina, Paris La Défense, France (JFR)
14.01.2004

1.13 REVIEWS

2.1 MELTING POINT

Value	:	= 178.7 °C
Sublimation	:	
Method	:	other: calculated using EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di(tert-dodecyl) pentasulphide (CAS Number 31565-23-8)
Method	:	MPBPWIN (v 1.40) Selected Melting Point (Weighted Value)
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

04.03.2004 (1)

Value	:	< 0 °C
Sublimation	:	
Method	:	other: no data
Year	:	
GLP	:	no data
Test substance	:	other TS
Test substance	:	TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0
Source	:	Atofina, Paris-La Défense, France.
Reliability	:	(4) not assignable

07.01.2004 (2)

Value	:	= -23 °C
Sublimation	:	
Method	:	other: no data
Year	:	
GLP	:	
Test substance	:	other TS
Test substance	:	TPS20, DITERTIODODECYL TRISULPHIDE, CAS no. 68425-15-0
Source	:	Atofina, Paris-La Défense, France.
Reliability	:	(4) not assignable

07.01.2004 (3)

2.2 BOILING POINT

Value	:	= 463.6 °C at
Decomposition	:	
Method	:	other: calculated using EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di(tert-dodecyl) pentasulphide (CAS Number 31565-23-8)
Method	:	MPBPWIN (v 1.40) Boiling Point (Adapted Stein and Brown Method)
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

04.03.2004 (1)

Value : > 200 °C at 1013 hPa
Decomposition : yes
Method : other: no data
Year :
GLP : no data
Test substance : other TS

Test substance : TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0
Source : Atofina, Paris-La Défense, France.
Reliability : (4) not assignable
07.01.2004 (2)

Value : > 200 °C at
Decomposition :
Method : other: no data
Year :
GLP :
Test substance : other TS

Test substance : TPS20, DITERTIODODECYL TRISULPHIDE, CAS no. 68425-15-0
Source : Atofina, Paris-La Défense, France.
Reliability : (4) not assignable
07.01.2004 (3)

2.3 DENSITY

Type :
Value : .95 g/cm³ at 20 °C
Method : other: no data
Year :
GLP :
Test substance : other TS

Source : Atofina, Paris-La Défense, France.
Test substance : TPS20, DITERTIODODECYL TRISULPHIDE, CAS no. 68425-15-0
Reliability : (4) not assignable
07.01.2004 (3)

Type : density
Value : = 1.01 g/cm³ at 20 °C
Method : other: no data
Year :
GLP : no data
Test substance : other TS

Source : Atofina, Paris-La Défense, France.
Test substance : TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0
Reliability : (4) not assignable
07.01.2004 (2)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : = .0000000076 hPa at 25 °C

Decomposition	:	
Method	:	other (calculated): EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di(tert-dodecyl) pentasulphide (CAS Number 31565-23-8)
Method	:	MPBPWIN (v 1.40) Selected Vapor Pressure (Modified Grain Method)
Remark	:	7.6E-9 hPa = 5.7E-9 mmHg
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

04.03.2004 (1)

Value	:	< .01 hPa at 20 °C
Decomposition	:	
Method	:	other (calculated): no data
Year	:	
GLP	:	no data
Test substance	:	other TS
Test substance	:	TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0
Source	:	Atofina, Paris-La Défense, France.
Reliability	:	(4) not assignable

07.01.2004 (2)

Value	:	< .1 hPa at 20 °C
Decomposition	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS
Test substance	:	TPS20, DITERTIODODECYL TRISULPHIDE, CAS no. 68425-15-0
Source	:	Atofina, Paris-La Défense, France.
Reliability	:	(4) not assignable

07.01.2004 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	
Log pow	:	= 11.86 at °C
pH value	:	
Method	:	other (calculated): EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Method	:	WSKOW v 1.40 Estimated Log Kow.
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Test substance	:	di(tert-dodecyl) pentasulphide (CAS Number 31565-23-8)
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

05.12.2003 (1)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	
Value	:	< 0 mg/l at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	insoluble (< 0.1 mg/L)
Stable	:	
Deg. product	:	
Method	:	other: calculated using EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di(tert-dodecyl) pentasulphide (CAS Number 31565-23-8)
Method	:	WSKOW v 1.40 Water Solubility.
Result	:	Calculated Water Solubility = 5.368E-8 mg/L
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

04.03.2004 (1)

Solubility in	:	Water
Value	:	at 20 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	not soluble
Stable	:	
Test substance	:	TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0
Source	:	Atofina, Paris-La Défense, France.
Reliability	:	(4) not assignable

07.01.2004 (2)

Solubility in	:	Water
Value	:	at °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	not soluble
Stable	:	
Deg. product	:	
Method	:	other: no data
Year	:	
GLP	:	
Test substance	:	other TS
Test substance	:	TPS20, DITERTIODODECYL TRISULPHIDE, CAS no. 68425-15-0
Source	:	Atofina, Paris-La Défense, France.
Reliability	:	(4) not assignable

07.01.2004 (3)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value : >= 121 °C
Type : closed cup
Method : other: ASTM D 93
Year :
GLP : no data
Test substance : other TS

Source : Atofina, Paris-La Défense, France.
Test substance : TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0
Reliability : (4) not assignable
07.01.2004 (2)

Value : > 121 °C
Type : closed cup
Method : other: ASTM D 93
Year :
GLP :
Test substance : other TS

Source : Atofina, Paris-La Défense, France.
Test substance : TPS20, DITERTIODODECYL TRISULPHIDE, CAS no. 68425-15-0
Reliability : (4) not assignable
07.01.2004 (3)

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

Result : flammable
Method :
Year :
GLP :
Test substance : other TS

Source : Elf Aquitaine Lacq
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0
Reliability : (4) not assignable
07.01.2004

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

Value : - 603 mPa s (dynamic) at 20 °C
Result :
Method :
Year :
GLP :
Test substance : other TS

Source : Atofina, Paris-La Défense, France.
Test substance : TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0
Reliability : (4) not assignable
07.01.2004 (2)

Value : 54 - 74 mPa s (dynamic) at 50 °C
Result :
Method :
Year :
GLP :
Test substance : other TS

Source : Atofina, Paris-La Défense, France.
Test substance : TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0
Reliability : (4) not assignable
07.01.2004 (2)

Value : - 7.9 mPa s (dynamic) at 100 °C
Result :
Method :
Year :
GLP :
Test substance : other TS

Source : Atofina, Paris-La Défense, France.
Test substance : TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0
07.01.2004 (2)

Value : - 207.7 mPa s (dynamic) at 20 °C
Result :
Method : other: no data
Year :
GLP :
Test substance : other TS

Source : Atofina, Paris-La Défense, France.
Test substance : TPS20, DITERTIODODECYL TRISULPHIDE, CAS no. 68425-15-0
Reliability : (4) not assignable
07.01.2004 (3)

Value : - 53 mPa s (dynamic) at 40 °C
Result :
Method : other: no data
Year :
GLP :
Test substance : other TS

Source : Atofina, Paris-La Défense, France.
Test substance : TPS20, DITERTIODODECYL TRISULPHIDE, CAS no. 68425-15-0
07.01.2004 (3)

Value : 22 - 34 mPa s (dynamic) at 50 °C

Result	:	
Method	:	other: no data
Year	:	
GLP	:	
Test substance	:	other TS
Source	:	Atofina, Paris-La Défense, France.
Test substance	:	TPS20, DITERTIODODECYL TRISULPHIDE, CAS no. 68425-15-0
Reliability	:	(4) not assignable

07.01.2004 (3)

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	**other**
Light source	:	
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
Deg. product	:	
Method	:	other (calculated): EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di(tert-dodecyl) pentasulphide (CAS Number 31565-23-8)
Method	:	AOP v 1.90: Hydroxyl Radicals.
Result	:	Overall OH Rate Constant = 683.5465 E-12 cm3/molecule-sec Half-Life = 0.016 Days (12-hr day; 1.5E6 OH/cm3) Half-Life = 11.266 Min
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions
Flag	:	Critical study for SIDS endpoint

05.12.2003 (1)

3.1.2 STABILITY IN WATER

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	**fugacity model level III**
Media	:	other: air-water-soil-sediment
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: EPIWIN v 3.10
Year	:	2003
Method	:	Used EPIWIN v 3.10. The following physical properties were used as the model input parameters: Chem Name: Di-tertiary-dodecyl pentasulfide Molecular Wt: 498.97 Henry's LC: 2.27 atm-m3/mole (Henrywin program) Vapor Press: 5.7E-9 mm Hg (Mpbpwin program) Liquid Vapor Press: 1.89E-7 mm Hg (super-cooled) Melting Pt: 179 deg C (Mpbpwin program)

Log Kow: 11.9 (Kowwin program)
Soil Koc: 2.97E+11 (calc by model)

Result : Results are provided in the following format:
Compartment / 100% to Air / 100% to Water / 100% to Soil / Equally to Each Compartment

Air / 4.35% / 5.23E-9% / 6.99E-8% / 0.00323%
Water / 0.346% / 1.87% / 0.0021% / 1.27%
Soil / 77.1% / 3.67E-9% / 99.9% / 31.9%
Sediment / 18.2% / 98.1% / 0.11% / 66.9%

Air: half life = .3756 hr; emissions = 1000 kg/hr
Water: half life = 3600 hr; emissions = 1000 kg/hr
Soil: half life = 3600 hr; emissions = 1000 kg/hr
Sediment: half life = 1.44E+4 hr; emissions = 0 kg/hr

Persistence when distributed equally to each compartment = 5.5E+3 hr (Emissions (kg/hr) = 1000 to air, 1000 to water, 1000 to soil, and 0 to sediment)

Source : EPI Suite v 3.10.
Chevron Phillips Chemical Company LP The Woodlands, TX

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
08.12.2003 (1)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

Type : **aerobic**
Inoculum : other: river water
Concentration : 800 mg/l related to Test substance
related to
Contact time : 28 day(s)
Degradation : = 0 (±) % after 28 day(s)
Result : under test conditions no biodegradation observed
Kinetic of testsubst. : 7 day(s) < 0 %
14 day(s) < 0 %
22 day(s) < 0 %
28 day(s) < 0 %
%
Control substance : Benzoic acid, sodium salt
Kinetic : 7 day(s) = 35.9 %
28 day(s) = 52.4 %
Deg. product : not measured
Method : Directive 84/449/EEC, C.3 "Biotic degradation - modified OECD screening test"
Year :
GLP : no data
Test substance : other TS

Test substance : Test compound: TPS 32
Chemical name: di-t-dodecyl polysulfide
CAS no.: 31565-23-8
Source: ATOCHEM

Batch: 6252
Sulfur content: no data

Test condition : INOCULUM/TEST ORGANISM
- Type of sludge: From river water
- Source: river water
- Sampling site: Levallois
- Preparation of inoculum: Water was deducted from the river, decantated and filtred on a 0.22µm filter.The filter was rinsed with water and introduced for sowing flasks.
- Initial cell concentration: 50µl/l

TEST SYSTEM
- Culturing apparatus: 300ml Erlenmeyer flask.
- Number of culture flasks per concentration: 10.
- Aeration device:the solution was saturated with compressed air for 6 hours.
- Closed vessels used: Yes.

INITIAL TEST SUBSTANCE CONCENTRATION: 800mg/l.
METHOD OF PREPARATION OF TEST SOLUTION: The substance was insoluble so it was introduced with acetone solvent which was evaporated before the test.

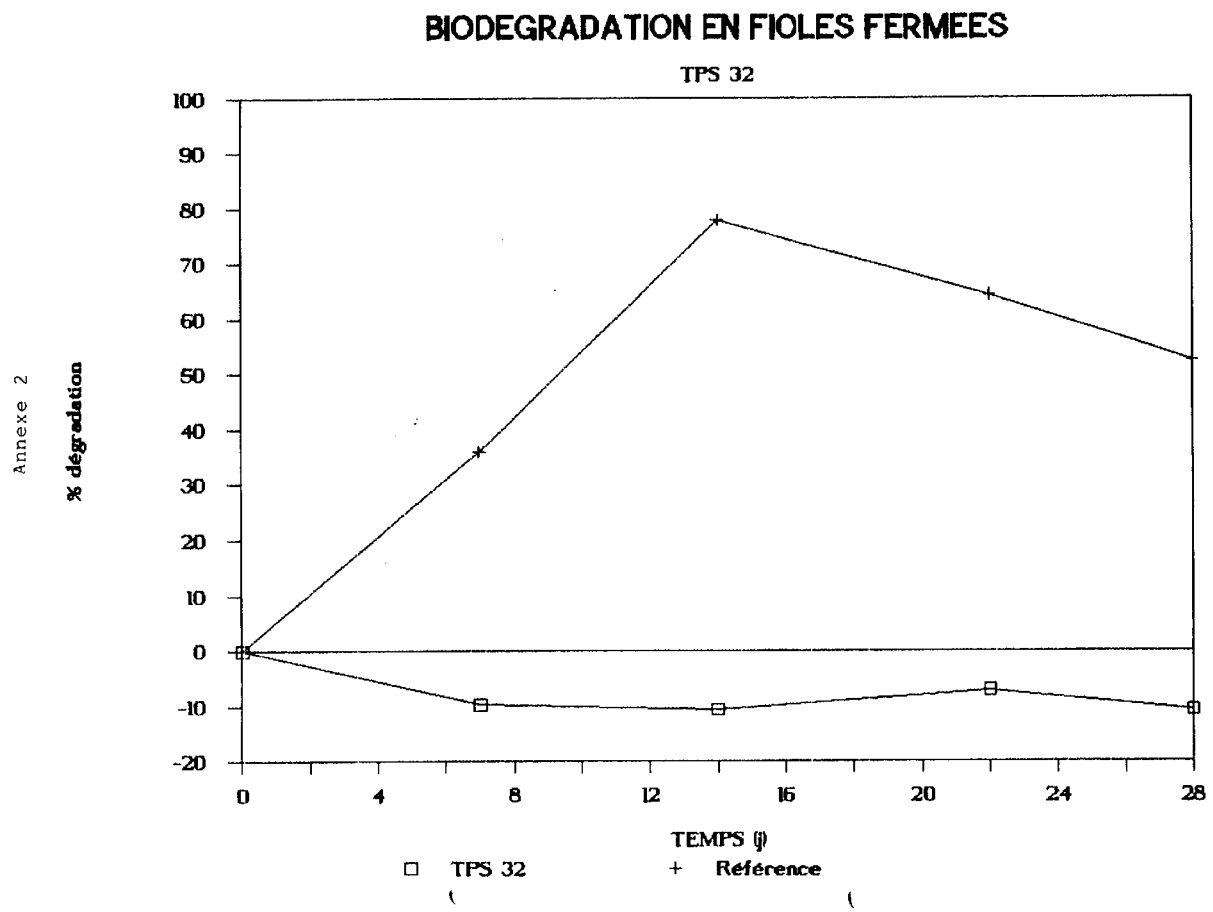
DURATION OF THE TEST: 28 days.

ANALYTICAL PARAMETER: The bacterial activity is evaluated by the consumption of dissolved O2, and the degradation follows from the difference between its consumption in flasks containing test substance and check flasks.
SAMPLING: 7, 14, 21, 28 days.

TEST CONDITIONS
- Composition of medium: For one litre of saturated water(with O2):
1- 1ml of solution a: KH2PO4 8.50g
K2HPO4 21.75g
Na2HPO4 33.40g
H2O 1 litre.
2- 1ml of solution b: NH4Cl 0.5g
H2O 1 litre.
3- 1ml of solution c: CaCl2 27.5g
H2O 1 litre.
4- 1ml of solution d: MgSO4,7H2O 22.50 g
H2O 1 litre.
5- 1ml of solution e: FeCl3 0.25g
E.D.T.A 0.40g
H2O 1 litre.
6- water q.s.p 1000 ml.

- Additional substrate: No.
- Test temperature: 21+/-1°C
INTERMEDIATES / DEGRADATION PRODUCTS: Not identified.
NITRATE/NITRITE MEASUREMENT: No.
REFERENCE SUBSTANCE: Benzoic acid,sodium salt.

Attached document : Courbe TPS 32.bmp



Conclusion	:	No degradation of TPS 32 was observed under the test conditions.
Source	:	ATOFINA, PARIS-LA-DEFENSE, FRANCE.
Reliability	:	(1) valid without restriction
Flag	:	Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

16.04.2004 (4)

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

BCF	:	= 3.16
Elimination	:	
Method	:	other: calculated using EPIWIN v 3.10
Year	:	2003
GLP	:	no
Test substance	:	other TS
Test substance	:	di(tert-dodecyl) pentasulphide (CAS Number 31565-23-8)
Method	:	Calculated using BCF Program (v 2.14).
Remark	:	Estimated Log BCF = 0.500
		Estimated Koc = 1.9E+7 (using PCKOC Program v 1.66)
Source	:	EPI Suite v 3.10. Chevron Phillips Chemical Company LP The Woodlands, TX
Reliability	:	(2) valid with restrictions

15.12.2003 (1)

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	yes
Method	:	OECD Guide-line 202
Year	:	1984
GLP	:	yes
Test substance	:	other TS
Test substance	:	Test compound: TPS 32 Chemical name: di-t-dodecyl polysulfide CAS no.: 31565-23-8 Source: ELF ATOCHEM Batch: 1209/98 Sulfur content: no data Appearance: yellow liquid or colourless Insoluble in water
Test condition	:	TEST ORGANISMS - Strain: Daphnia magna straus strain 5 or A. - Source/supplier: Breeding colony was realized in Elendt M7 medium in the laboratory, organisms were selected by sieving. - Breeding method: Not available. - Age: Less than 24 hours. - Feeding: Microscopic algae Raphidocelis subcapitata. - Pretreatment: No. - Feeding during test: No. - Control group: Yes. STOCK AND TEST SOLUTION AND THEIR PREPARATION - Preparation: Since TPS 32 is poorly soluble in water; a saturated solution was prepared by vigorously mixing: -100 mg of TPS 32 with dilution water during 23 hours at 20°C (preliminary test). - 2 mg of TPS 32 with dilution water during 68 hours at 20°C (definitive test). After this saturation period, the saturated solution was filtered with a HV 0.45 µm filter. - Vehicle, solvent: Ultrapure water. STABILITY OF THE TEST CHEMICAL SOLUTIONS: Not available, because the analytical method did not allow the determination of the test substance concentration. REFERENCE SUBSTANCE: Potassium dichromate. DILUTION WATER: was prepared in the laboratory using pure water and salts according to ISO 6341. For one litre: 25 ml of the below solutions 1- 11.76g CaCl2,2H2O/l ultrapure water. 2- 4.93g MgSO4,7H2O/l ultrapure water. 3- 2.59g NaHCO3/l ultrapure water. 4- 0.23g KCl/l ultrapure water.

- Aeration: aerated up until oxygen saturation.
- Ca/Mg ratio: 4.
- Na/K ratio: 10.

TEST SYSTEM
- Concentrations: 6.25, 12.5, 25, 50, 100 nominal concentration (% vol), forming a geometric progression with a factor of 2.
- Renewal of test solution: No.
- Exposure vessel type: 120 ml closed flasks with butyl rubber caps covered with PTFE.
- Number of replicates: 4.
- Number of individuals per replicate: 5 daphnids by replicate.
- Test temperature: 19-21°C.
- Dissolved oxygen: >2 mg/l.
- pH: 7.69-8.07.
- Adjustment of pH: No.
- Photoperiod: Incubation of test flasks in darkness.

DURATION OF THE TEST: 24 and 48 hours.
TEST PARAMETER: The percentage of daphnids immobilisation after 24 and 48 hours.
SAMPLING: 24, 48 hours.
MONITORING OF TEST SUBSTANCE CONCENTRATION: HPLC/MS.

Result : At the solubility limit of the test substance, no significative immobilization of the test organisms was recorded after 24 and 48 hours.

Thus the TPS 32 was not toxic for daphnia at the maximal exposure concentration corresponding to the solubility limit of the TPS 32 in the test medium.

The solubility limit of TPS 32 in the test medium was below the range of quantification (i.e.0.1 mg/l) and above the detection limit (i.e.0.02 mg/l) of the analytical method.

0.03 mg/l < Solubility limit <0.1 mg/l

- Nominal/measured concentrations: Attached document.
- Effect data (Immobilisation): Attached document.

RESULTS TEST WITH REFERENCE SUBSTANCE: The sensibility of the biologic reactive is controlled by a toxicity test with Potassium dichromate periodically, EC50/24h =1.1mg/l.

Attached document : Results TPS 32.bmp

6.1. Essai définitif

Le tableau ci-dessous présente les pourcentages d'immobilisation à 24h et 48h ainsi que les résultats des analyses chimiques réalisées par la méthode présentée en annexe 3.

Concentration				Immobilisation	
Nominale	Mesurée				
vol. solution. saturée (%)	Initiale (mg/l)	Finale (mg/l)	Final/Initial %	à 24 h (%)	à 48 h (%)
100	< LQ et > LD	< LQ et > LD	-	5	5
50	< LD	< LD	-	0	5
25	NA	NA	-	0	0
12,5	NA	NA	-	5	5
6,25	NA	NA	-	0	0

LQ : Limite de Quantification de la méthode d'analyse soit 0,1 mg/l.
LD : Limite de Détection de la méthode d'analyse soit 0,03 mg/l.
NA : concentration non analysée.

Remark : The method was applied with respect to its quality criteria:
- Immobilisation in the control did not exceed 10% at the end of the test.
- Concentration of dissolved oxygen in the test vessels remained above 2 mg/l at the end of the test.
- pH did not vary by more than 1 unit.

The solubility of the test substance in the test medium was below the limit of quantification of the analytical method. Therefore the stability of the substance during the assay has not been checked.

Source : ATOFINA, PARIS-LA-DEFENSE, FRANCE.
Reliability : (1) valid without restriction
Flag : Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

16.04.2004 (5)

Type : static
Species : Daphnia magna (Crustacea)
Exposure period : 48 hour(s)
Unit : mg/l
Analytical monitoring : yes
Method : OECD Guide-line 202
Year : 1984
GLP : yes
Test substance : other TS

Test substance : Test compound: TPS 32
Chemical name: di-t-dodecyl polysulfide
CAS no.: 31565-23-8
Source: ELF ATOCHEM
Batch: 4352-96
Sulfur content: no data
Appearance: yellow liquid or colourless
Solubility: slightly soluble in water.

Test condition : TEST ORGANISMS
- Strain: Daphnia magna straus strain 5 or A.
- Source/supplier: Breeding colony was realized in Elendt M7 medium in the laboratory, organisms were selected by sieving.
- Breeding method: Not available.
- Age: Less than 24 hours.
- Feeding: Microscopic algae Raphidocelis subcapitata.
- Pretreatment: No.

- Feeding during test: No.
- Control group: Yes.

STOCK AND TEST SOLUTION AND THEIR PREPARATION
- Preparation: Since TPS is poorly soluble in water; 3 saturated solution were prepared by vigorously mixing:
-1, 10, 100 mg of TPS 32 with dilution water during 24 hours at 20°C. After this saturation period, the saturated solutions were centrifuged at 20°C, 2000g, during 20 mn.
- Vehicle, solvent: Ultrapure water.

STABILITY OF THE TEST CHEMICAL SOLUTIONS: Not available, because the analytical method did not allow the determination of the test substance concentration.

REFERENCE SUBSTANCE: Potassium dichromate.

DILUTION WATER: was prepared in the laboratory using pure water and salts according to ISO 6341.
For one litre: 25 ml of the below solutions
1- 11.76g $CaCl_2,2H_2O$/l ultrapure water.
2- 4.93g $MgSO_4,7H_2O$/l ultrapure water.
3- 2.59g $NaHCO_3$/l ultrapure water.
4- 0.23g KCl/l ultrapure water.
- Aeration: aerated up until oxygen saturation.
- Ca/Mg ratio: 4.
- Na/K ratio: 10.

TEST SYSTEM
- Concentrations: 1, 10, 100 mg/l.
- Renewal of test solution: No.
- Exposure vessel type: 120 ml closed flasks with butyl rubber caps covered with PTFE.
- Number of replicates: 4.
- Number of individuals per replicate: 5 daphnids by replicate.
- Test temperature: 19-21°C.
- Dissolved oxygen: >2 mg/l.
- pH: 8.07-8.14.
- Adjustment of pH: No.
- Photoperiod: Incubation of test flasks in darkness.

DURATION OF THE TEST: 24 and 48 hours.
TEST PARAMETER: The percentage of daphnids immobilisation after 24 and 48 hours.
SAMPLING: 24, 48 hours.

MONITORING OF TEST SUBSTANCE CONCENTRATION: HPLC/MS

Result **:** The percentage of immobilisation are presented in the following table for each of the 3 tested concentrations:

Mesured concentration		% of Immobilisation	
T0	T48	T0	T48
1.9	NA	5	100
0.31	NA	0	85
ND	NA	0	0

At the nominal concentration of 10mg/l, corresponding to a measured concentration of 0.31 mg/l, 85% of daphnids were immobilised.
Visual observations on the test solutions at nominal concentrations of 10 and 100 mg/l showed that the solubility limit of TPS 32 is probably lower than 0.31 mg/l.

Therefore the toxic effect of 85% may result from micro drops of non-solubilized test substance.

At the nominal concentration of 1mg/l, no toxicity was recorded and TPS 32 was not quantified since its concentration was below the detection limit of the analytical method i.e.0.04 mg/l.

Remark : In accordance with the study monitor, no analyse was performed at the end of the test.

Thus the quality criteria related to the stability of the substance all along the test duration has not been checked. Therefore, RESULTS OF THIS STUDY SHOULD BE INTERPRETED WITH CAUTION.

Source : ATOFINA, PARIS-LA-DEFENSE, FRANCE.
Reliability : (4) not assignable
Flag : Directive 67/548/EEC
16.04.2004 (6)

Type :
Species : Daphnia magna (Crustacea)
Exposure period : 24 hour(s)
Unit : mg/l
EC0 : < .035
EC50 : = .449
EC100 : = 3.11
Analytical monitoring : no
Method : other: AFNOR NF T 90-301
Year :
GLP : no
Test substance : no data

Result : EC50,24h = 0.449 mg/l
EC50,24h corrected = 0.514 mg/l

EC100,24h = 3.11 mg/l
EC0,24h <0.035 mg/l

More informations:
At the concentration of 0.35 mg/l: pH = 7.89
At the concentration of 0.69 mg/l: pH = 7.80

Remark : The test was performed in presence of acetone as a solvent.
Source : Atofina, Paris-la-Défense, France.
Reliability : (4) not assignable
16.04.2004 (7)

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : **other algae: Pseudokirchneriella Subcapitata**
Endpoint : growth rate
Exposure period : 72 hour(s)
Unit : mg/l
Limit test : no
Analytical monitoring : yes
Method : OECD Guide-line 201 "Algae, Growth Inhibition Test"
Year : 1984
GLP : yes
Test substance : other TS

Test substance : Test compound: TPS 32
Chemical name: di-t-dodecyl polysulfide
CAS no.: 31565-23-8

Source: ELF ATOCHEM
Batch: 507/99
Sulfur content: no data
Appearance: yellow liquid or colourless
Insoluble in water

Method : - Analytical device:
pHmeter Mettler Toledo 345, Oxymeter WTW 538, Optical Microscope Zeiss RA34, Cytofluor 2350 microplate reader.

- Statistical test: Dunnett test.

Test condition : TEST ORGANISMS
- Strain: CCAP 278/4.
- Source/supplier: Culture Centre of Algae and Protozoa
- Method of cultivation: Parent cell suspensions were subcultured every week in 100 ml flasks, incubated at 23 ± 1°C, with alternative lighting (16h light / 8h darkness), under continuous aeration with filtrated Air (0.22µm).
- Pretreatment: 4 days before treatment, parent cultures are diluted (5 ml in 500 ml) to prepare 2 pre-cultures (one for sowing, the other for rescue).
- Controls: Quality of parent cultures was checked under a microscope to verify the absence of microorganisms or deformed cells.
- Initial cell concentration: 10000 cells/ml.

STOCK AND TEST SOLUTION AND THEIR PREPARATION
- Preparation: Since TPS is poorly soluble in water; a saturated solution was prepared by vigorously mixing 100 mg of TPS 32 with 1 litre of dilution water during 24 hours (this solution was agitated at 30°C for 3 hours and then at 23°C for 21 hours).
After this saturation period, droplets were observed on glass and in suspension in water. The saturated solution was filtered with a 0.22 µm filter.

- Vehicle, solvent: dilution water described below (in "Growth test medium chemistry") completed with NaHCO3 (0.3 g/l) and Hepes buffer state (6mM).

STABILITY OF THE TEST CHEMICAL SOLUTIONS: Not available, the concentration of TPS 32 in the saturated solution was not determined since it was assessed as below the detection limit of the analytical method.

REFERENCE SUBSTANCE:
Current method (C3, described in Directive 92/69/EEC) does not require a test with K2Cr2O7 as a quality criterion. However, the sensibility of the biologic reactive is controlled by a toxicity test with K2Cr2O7 every 2 months.

DILUTION WATER: was prepared by mixing ultrapure water with specific volume of the following solutions described below in Growth test medium.
-PH: 8 after equilibration with Air.
-Temperature: Dilution water must be preserved just for a few days at 23+/-2°C in darkness.

GROWTH TEST MEDIUM CHEMISTRY
Solution 1: Macronutriments
- NH4Cl : 15 mg/l
- MgCl2.6 H2O: 12 mg/l
- CaCl2.2 H2O: 18 mg/l
- MgSO4.7 H2O: 15 mg/l
- KH2PO4 : 1.6 mg/l

Solution 2: Fe-EDTA
- FeCl3.6 H2O: 0.08 mg/l

- Na2 EDTA.2 H2O: 0.1 mg/l

Solution 3: Oligoelements
- H3BO3 : 0.185 mg/l
- MnCl2.4 H2O : 0.415 mg/l
- ZnCl2 : 3x10-3 mg/l
- CoCl2.6 H2O : 1.5x10-3 mg/l
- CuCl2.2 H2O : 10-5 mg/l
- Na2MoO4.2 H2O : 7x10-3 mg/l

Solution 4: NaHCO3
- NaHCO3: 50 mg/l

TEST SYSTEM
- Test type: phytoculture chamber with rotating trays.
- Renewal of test solution: No.
- Exposure vessel type: 120 ml glass bottles stoppered with PTFE bungs and sealed with aluminium caps.
- Number of replicates per dose: 3.
- Concentrations: 9.39, 20.66, 45.45, 100 nominal concentration (% vol)forming a geometric progression with a factor of 2.2.
- Test temperature: 24 ± 1°C
- Intensity of irradiation: No data.
- Photoperiod: 16h light / 8h darkness.

pH and dissolved oxygen were measured at the beginning and the end of the test in the test solutions.

concentration nominale %vol	pH T0	pH T72h	Dissolved O2 T0	Dissolved O2 T72h
0	7.58	7.61	9.3	10
9.39	7.19	7.64	9.2	10.5
20.66	7.19	7.68	9.2	10.1
45.45	7.16	7.68	9.1	10.1
100	7.17	7.62	9.0	10.2

TEST PARAMETER: Inhibition of cellular multiplication.

MONITORING OF TEST SUBSTANCE CONCENTRATION: HPLC/MS.

Result : TPS 32 has a solubility limit of 0.080 mg/l in dilution water.

The results of this study show that NO INHIBITION OF GROWTH was observed after 72 hours of exposure to the saturated stock solution of TPS 32.

Growth curve: Attached document.

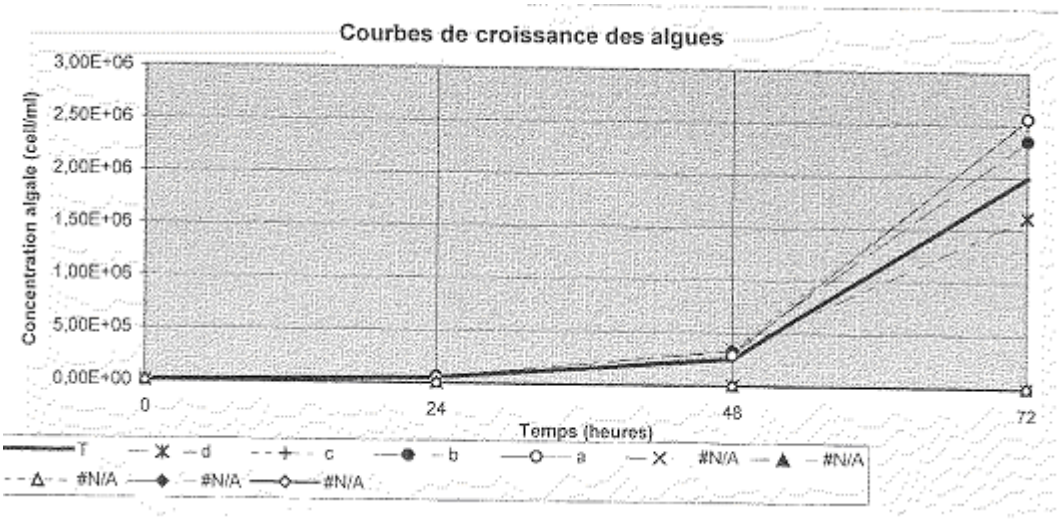
Cell density data: Attached document.
-A: Area under the curve
-µ: Growth rate

Inhibition percentages IA and Iµ: Attached document
IA: inhibition percentage based on Biomass.
Iµ: inhibition percentage based on Growth rate.

Attached document : TPS 32 A&µ.bmp
TPS 32 curve algae.bmp

Echantillon Référence	Concentration nominale (% Vol)	Concentration algale moyenne (cellules/ml) T0	T24h	T48h	T72h	$\bar{A}$	$\bar{\mu}$
T	0	10^4	$5,27\ 10^4$	$2,51\ 10^5$	$2,00\ 10^6$	$3,06\ 10^7$	0,0736
d	9,39	10^4	$5,47\ 10^4$	3,35 105	$1,62\ 10^6$	$2,82\ 10^7$	0,0707
c	20,66	10^4	$6,10\ 10^4$	$3,36\ 10^5$	$2,55\ 10^6$	$3,95\ 10^7$	0,0769
b	45,45	10^4	$6,10\ 10^4$	$3,29\ 10^5$	$2,35\ 10^6$	$3,70\ 10^7$	0,0758
a	100	10^4	$5,40\ 10^4$	$2,89\ 10^5$	$2,56\ 10^6$	$3,84\ 10^7$	0,0770

A: area under the curve
μ: growth rate



Remark : Study Peer Reviewed.
The appearance of the test solutions was visually checked at the beginning and the end of the test. Solutions were found to be clear. No precipitation was observed at the end of the test.

Microscopic observation confirmed that the algae appeared normal at the end of the test. The normal form of the unicellular algae is a crescent shaped cell with an average length of 5-10 µm.

QUALITY CRITERIA:
During the test the control pH varied by 0.52 units.

-The validity criterion of the study related to the growth of algae was respected: the increase in cell density (R) measured during the test was greater than a factor of 16 (R = 200).

-The validity criterion specific to C3 92/69EEC method and related to the test item stability during the test was not verified:
The concentration of TPS 32 in the saturated solution was not determined since it was assessed as below the detection limit of the analytical method.

Source : ATOFINA, PARIS-LA-DEFENSE, FRANCE.
Reliability : (1) valid without restriction
Flag : Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

16.04.2004 (8)

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Type :
Species : Pseudomonas putida (Bacteria)
Exposure period : 16 hour(s)

Unit	:	mg/l
Method	:	other: Norme ISO/TC 147/SC 5 WG 1(N111)
Year	:	
GLP	:	yes
Test substance	:	other TS
Test substance	:	Test compound: TPS 32 Chemical name: di-t-dodecyl polysulfide CAS no.: 31565-23-8 Source: ATOCHEM Batch: 6252 Sulfur content: no data Appearance: yellow liquid Insoluble in water
Test condition	:	TEST ORGANISMS - Species: Pseudomonas Pituda MIGULA, Berlin 33/2. - Bacterial suspension: 50ml of solution I(described in the growth test medium)+ 125ml of solution II+ 50 ml of solution IV+ 18 g of Agar Gelose (microbiological use)+ Water q.s.p 1 litre. This mixture was sterilised at 120°C during 15 min. - Preculture medium: 25 ml solution I+25 ml solution III+50 ml solution IV. pH of this medium: 7.2+/-0.2. - Preparation: Inoculum was obtained from the preculture medium (less than 7 days), incubated during 7 hours for exponential phase growth. TEST SOLUTION: Since the TPS 32 was insoluble in water, 3 methods of introduction of TPS 32 were used: 1- TPS 32 was introduced directly in 100 ml of test medium by fractions from 10 mg to 1000mg. Flasks were placed under agitation during 16 hours at 21°C. 2- Formation of initial emulsion 5g/l of deionised water; by ultra sounds. Different dilutions of this emulsion were prepared until 1000mg/l. Flasks were placed under agitation during 16 hours at 21°C. 3- Dissolution of TPS 32 in DMF(diméthylformamide) forming an initial solution at 5g/l. In the different dilutions of this initial solution, the limit of DMF must be < 0.2% , above this limit the DMF have an inhibitory effect > 10% to bacteria. Flasks were placed under agitation during 16 hours at 21°C. REFERENCE SUBSTANCE: 3,5-dichlorophenol GROWTH TEST MEDIUM CHEMISTRY Solution I: NaNO3 10g K2HPO4 2.40g KH2PO4 1.20g Yeast 1g Water q.s.p 500ml Solution II: NaNO3 10g K2HPO4 2.40g KH2PO4 1.20g Water q.s.p 500ml Solution III: C6H12O6 solution C6H12O6,H2O 40g for biochemical and microbiological use Water q.s.p 500ml.

Solution IV:
MgSO4,7H2O 4g
Fe(III) citrate 0.01g, 19% Fe
Water q.s.p 1000ml

TEST SYSTEM
- Exposure vessel type: 250ml and 180 ml sterilised flasks.
- Test temperature: 21+/-1°C.
- Duration of the test: 16+/-1 hours.

TEST PARAMETER: Inhibition of cellular multiplication.
END POINT: Biomass, measured by Turbidity.

Result : It was not possible to detect an inhibitory effect of the substance towards Pseudomonas putida, in the 3 types of experiences.
The maximum concentration tested was 10 g/l.

*3,5 Dichlorophenol
CE50,16h = 18.3 mg/l.

Remark : Since the substance was insoluble in water, 3 types of experiences were realised:

- The test substance was directly put in culture medium.
- It was dispersed by ultra sounds.
- It was dissolved in dimethylformamide.

Study Peer Reviewed.

Source : ATOFINA, PARIS-LA-DEFENSE, FRANCE.
Reliability : (1) valid without restriction
Flag : Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

16.04.2004 (9)

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	**LD0**
Value	:	> 12.5 ml/kg bw
Species	:	mouse
Strain	:	Swiss
Sex	:	male
Number of animals	:	40
Vehicle	:	other: undiluted
Doses	:	
Method	:	other
Year	:	1973
GLP	:	no
Test substance	:	
Test substance	:	Test compound: TPS 32 Chemical name: di-t-dodecyl polysulfide CAS no.: 31565-23-8 Source: SNPA Batch: pure laboratory sample Sulfur content: no data
Test condition	:	The mortality was observed on a 7-day period. Clinical signs and body weight gain were not reported.
Source	:	Atofina, Paris-la-Défense, France.
Reliability	:	(2) valid with restrictions No additional details available.
Flag	:	Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

16.04.2004 (10)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type	:	**LD0**
Value	:	>= 2000 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	20
Vehicle	:	other: none
Doses	:	
Method	:	OECD Guide-line 402 "Acute dermal Toxicity"
Year	:	1981
GLP	:	yes
Test substance	:	
Test substance	:	Test compound: TPS 32 Chemical name: di-t-dodecyl polysulfide CAS no.: 31565-23-8 Source: SNEAP Batch: fabriquation Industrielle, no. 22463

		Sulfur content 30.53%
Result	:	CLINICAL EXAMINATIONS: No mortality and no behavioral anomaly were raised following the administration of the product and during the 14 following days. The local tolerance of the product was good: no cutaneous lesion (erythema or oedema) was raised at the site of application of the product during the observation period BODY WEIGHT GAIN: The body weight gain of the treated animals was not affected by the treatment. MACROSCOPIC EXAMINATIONS: No macroscopic abnormality was observed in the animals sacrificed at the end of the observation period.
Conclusion	:	The dermal LD0 of TPS 32 is higher than 2000 mg/kg.
Source	:	Atofina, Paris-la-Défense, France.
Reliability	:	(1) valid without restriction
Flag	:	Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

26.02.2004 (11)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

Species	:	rabbit
Concentration	:	undiluted
Exposure	:	Semiocclusive
Exposure time	:	4 hour(s)
Number of animals	:	6
Vehicle	:	
PDII	:	
Result	:	slightly irritating
Classification	:	not irritating
Method	:	OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
Year	:	1981
GLP	:	yes
Test substance	:	
Test substance	:	Test compound: TPS 32 Chemical name: di-t-dodecyl polysulfide CAS no.: 31565-23-8 Source: SNEAP Batch: fabriquation Industrielle, no. 22463 Sulfur content 30.53%
Result	:	TPS 32 produced a slight erythema in one rabbit and a moderate erythema in 5 rabbits. A slight oedema was observed in 3 rabbits. Mean score (24+48+72 h) - Erythema : 1.72 - Oedema : 0.39
Source	:	Atofina, Paris-la-Défense, France.
Reliability	:	(1) valid without restriction
Flag	:	Material Safety Dataset, Directive 67/548/EEC

26.02.2004 (12)

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	undiluted
Dose	:	.1 ml
Exposure time	:	24 hour(s)
Comment	:	not rinsed
Number of animals	:	6
Vehicle	:	
Result	:	slightly irritating
Classification	:	not irritating
Method	:	OECD Guide-line 405 "Acute Eye Irritation/Corrosion"
Year	:	1981
GLP	:	yes
Test substance	:	
Test substance	:	Test compound: TPS 32 Chemical name: di-t-dodecyl polysulfide CAS no.: 31565-23-8 Source: SNEAP Batch: fabriquation Industrielle, no. 22463 Sulfur content 30.53%
Result	:	TPS 32 incuced a slight chemosis and/or enanthema which persist for up to 72 hours in 2 animals. Slight iridal congestion was observed up to 48 hours in some animals. Mean scores (24 + 48 +72 h): - chemosis: 0.89 - Enanthema : 0.61 - Iris: 0.33 - Cornea: 0.00
Source	:	Atofina, Paris-la-Défense, France.
Reliability	:	(1) valid without restriction
Flag	:	Material Safety Dataset, Directive 67/548/EEC

26.02.2004 (13)

5.3 SENSITIZATION

Type	:	**Guinea pig maximization test**
Species	:	guinea pig
Concentration	:	1st: Induction 1 % intracutaneous 2nd: Induction undiluted occlusive epicutaneous 3rd: Challenge undiluted occlusive epicutaneous
Number of animals	:	30
Vehicle	:	
Result	:	ambiguous
Classification	:	not sensitizing
Method	:	OECD Guide-line 406 "Skin Sensitization"
Year	:	1986
GLP	:	yes
Test substance	:	
Test substance	:	Test compound: TPS 32 Chemical name: di-t-dodecyl polysulfide CAS no.: 31565-23-8 Source: SNEAP Batch: fabriquation Industrielle, no. 22463 Sulfur content 30.53%
Method	:	. The applications corresponding to "the induction" were

carried out
- By intradermal route : injection of 2 x 0.1 ml
* on one hand, with the test article in a 1 % (W/V) solution in water for, injection ;
* on the other hand, with the 50/50 (V/V) mixing : test article in a 2 % solution (W/V) in water for injection + complete Freund's adjuvant at 50 % (V/V) in isotonic injectable solution, i.e. a final 1 % concentration of the sample to control.

Injection of the test article in a 1 % solution has provoked a weak to moderate irritation.

- By topical occlusive route for 48 hours, with the test article as supplied and at the dose level of 0.5 ml per animal.
This application having not provoked any weak to moderate irritation, a skin painting was carried out on Day 8, with 0.5 ml of Sodium Lauryl Sulfate at 10 % in Codex liquid paraffin.

- During the "challenge exposure", the topical occlusive application for 24 hours was carried out with the test article as supplied and at the dose level of 0.5 ml per guinea-pig (Maximum Non-Irritant Concentration : M.N.I.C.).

Result : From the macroscopic and histological results obtained under the experimental conditions, it may be concluded that the test article has provoked an aspecific reaction of
irritation of weak intensity in 4 out of the 20 treated guinea-pigs, this phenomenon can hide possible weak reactions of cutaneous sensitization, no characteristic cutaneous abnormality and different from the preliminary study was noted in the 10 control guinea-pigs.

Source : Atofina, Paris-la-Défense, France.
Reliability : (1) valid without restriction
Flag : Material Safety Dataset, Directive 67/548/EEC
26.02.2004 (14)

5.4 REPEATED DOSE TOXICITY

Type :
Species : rat
Sex : male/female
Strain : Sprague-Dawley
Route of admin. : gavage
Exposure period : 28 days
Frequency of treatm. : daily
Post exposure period : 14 days
Doses : 50, 250, 1000 mg/kg/d
Control group : yes, concurrent vehicle
NOAEL : = 1000 mg/kg bw
Method : Directive 84/449/EEC, B.7 "Sub-acute toxicity (oral)"
Year : 1992
GLP : yes
Test substance :

Test substance : Test compound: TPS 32
Chemical name: di-t-dodecyl polysulfide
CAS no.: 31565-23-8
Source: EAP

		Batch: 152319 (94_000858) Sulfur content 31.07%
Method	:	Two groups of six male and six female Sprague-Dawley rats received the TPS 32 daily by gavage at dose-levels of 50 or 250 mg/kg/day, and two groups of 12 males and 12 females was given 0 or 1000 mg/kg/day for four weeks. On completion of the four week treatment period, the first six surviving animals of each sex in the control and high dose groups were kept for a two week recovery period. Clinical signs and mortality were checked daily. Body weight and food comsumption were recorded once a week. Haematological and blood biochemical examinations and urinalysis were performed on week 5. At the end of the treatment period, all the surviving animals were killed and a macroscopic examination was performed. Designated organs were weighed and representative tissues specimen were submitted to a microscopic examination.
Result	:	No deaths related to the treatment occurred during the treatment period or the recovery period. Ptyalism was observed in all the animals of both sexes given 1000 mg/kg/day during the treatment period. Thereafter, during the recovery period, no clinical signs were observed. During the treatment and the recovery periods, the mean food consumption and body weight gain were similar between treated and control animals. No abnormalities of toxicological importance were noted among haematological and blood biochemical parameters, urinalysis, organ weights, macro- and microscopic examinations.
Conclusion	:	The No Observable Adverse Effect Level (NOAEL) was defined as 1000 mg/kg/day.
Source	:	Atofina, Paris-la-Défense, France.
Reliability	:	(1) valid without restriction
Flag	:	Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

26.02.2004 (15)

Type	:	
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	8 days
Frequency of treatm.	:	daily
Post exposure period	:	none
Doses	:	50, 250, 1250 and 2500 mg/kg
Control group	:	yes, concurrent vehicle
NOAEL	:	= 1250 mg/kg bw
LOAEL	:	2500 mg/kg bw
Method	:	other: range-finding study
Year	:	
GLP	:	no
Test substance	:	other TS
Test substance	:	Test compound: TPS 32 Chemical name: di-t-dodecyl polysulfide CAS no.: 31565-23-8 Source: EAP Batch: 94_000670 Sulfur content 31.07%
Method	:	Four groups of 4 male and 4 female Sprague-Dawley rats received the TPS 32 daily by gavage at doses of 0, 50, 250, 1250 and 2500 mg/kg/day for 8 days. Clinical signs and mortality were checked twice daily. Food comsumption and

body weight were recorded twice a week. A complete macroscopic examination was performed on all animals killed at the end of the study. Adrenals, heart, kidneys, liver, spleen, thymus and gonades were weighed on all animals.

Result : No mortality occured during the treatment period. Ptyalism was observed in all the males given 1250 or 2500 mg/kg/day and in 2/4 or 3/4 females given 1250 or 2500 mg/kg/day, respectively. A slightly lower mean food consumption and body weight gain was observed in the males given 2500 mg/kg/d. Thickened and/or translucent wall of forestomach was noted for 3/4 females given 2500 mg/kg/day. No effect of treatment was observed on organ weights.

Source : Atofina, Paris-la-Défense, France.

Reliability : (2) valid with restrictions

26.02.2004 (16)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : **Salmonella typhimurium reverse mutation assay**
System of testing : Strains : TA 98, TA 100, TA 1535, TA 1537, TA 1538
Test concentration : 0, 5, 150, 500, 150, 5000 µg/plate
Cycotoxic concentr. : >= 5000 µg/plate
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 471
Year : 1986
GLP : yes
Test substance :

Test substance : Test compound: TPS 32
Chemical name: di-t-dodecyl polysulfide
CAS no.: 68425-16-1
Source: SNEA(P)
Batch: 2246
Sulfur content: no data

Test condition : SYSTEM OF TESTING
- 2 independent trials; the direct plate incorporation method was used with and without métabolic activation (MA). 3 plates per concentration
- Metabolic activation system (MA): S9 fraction from liver homogenates of rats induced with 500 mg/kg Aroclor 1254
- solvent: ethanol
- Controls: . solvent control (with and without MA)
. Positives controls:
- Without S9
2-nitrofluorene: TA 98, 1.0 µg/plate; TA 1538, 2 µg/plate
ENNG: TA100, 3.0 µg/plate; TA 1535, 5 µg/plate
9-aminoacridine: TA1537, 80 µg/plate
- With S9
2-aminoanthracene: TA98, TA100 and TA1538, 0.5 µg/plate; TA 1535 and TA1535, 2 µg/plate
. sterility control checked during the test.
- Concentrations: 5, 150, 500, 150, 5000 µg/plate
- Cytotoxicity: A preliminary toxicity test was performed to define the concentrations to be used for the mutagenicity study. All strains exposed to 5-5000 µg/plate with and without MA

CRITERIA FOR EVALUATION
- negative and positive controls within the range of historical controls.
- positive: reproducible and significant dose related increase in revertants and/or reproducible doubling in the number of revertants compared with

negative controls for one dose.

Result : TPS-32 was not toxic towards the tester strains. Therefore 5000 µg/plate was chosen as the top dose level in the mutation tests.

No substantial increases in revertant colony numbers of any of the five tester strains were observed following treatment with TPS-32 at any dose level, either in the presence or absence of metabolic activation (S-9 mix).

Source : Atofina, Paris-la-Défense, France.
Reliability : (1) valid without restriction
Flag : Material Safety Dataset, Critical study for SIDS endpoint
26.02.2004 (17)

Type : **Chromosomal aberration test**
System of testing : human lymphocytes
Test concentration : 0, 300, 1000, 2500 µg/ml
Cycotoxic concentr. : > 2500 µg/ml (limit of solubility)
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 473
Year : 1983
GLP : yes
Test substance :

Test substance : Test compound: TPS 32
Chemical name: di-t-dodecyl polysulfide
CAS no.: 31565-23-8
Source: SNEA(P)
Batch D59B
Sulfur content 30.14%.

Method : The test substance was tested with and without a metabolic activation system, the S9 mix, prepared from a liver microsomal fraction (S9) of rats induced with Aroclor 1254.

The conditions of treatment were as follows, using 2 cultures/experimental point:
. without S9 mix: the cultures were incubated with the test or control substances which remained in the culture medium, until the appropriate harvest times*: 24 and 48 hours

. with S9 mix: the test or control substances remained in a culture medium containing 15% S9 mix (10% S9/S9 mix) for 2 hours. The cells were then centrifuged, the treatment medium removed, the cells resuspended in fresh culture medium. The cultures were then incubated until the appropriate harvest times*: 24 and 48 hours.

Two hours before harvesting, the cells were treated with a colcemid solution to block them at the metaphase-stage of mitosis. The chromosomal preparations were stained and screened microscopically for mitotic index and for aberrations: 200 well-spread metaphases per concentration were read, whenever possible.

The concentrations of TPS 32 for scoring were: 300, 1000 and 2500 µg/ml, 2500 µg/ml being the limit of solubility of the test substance in the culture medium.

Positive controls: Mitomycin C (0.2 µg/ml) without S9, Cyclophosphamide (50 µg/ml) with S9.

A reproducible and statistically significant increase in the aberrant cells

frequency for at least one of the tested concentrations is considered as a positive response.

* after the beginning of treatment

Result	:	For the test, the aberrant cells frequency in the negative and vehicle controls was within the range of our historical data (i.e. 0.5 ± 0.6%, gaps excluded). The aberrant cells frequency in the positive controls was significantly higher ($p < 0.001$) than that of the negative controls, indicating the sensitivity of the test system. The test substance did not induce any significant increase in the aberrant cells frequency, with or without S9 mix, for both of the 2 harvest times.
Conclusion	:	TPS 32 did not show clastogenic activity in this chromosomal aberration test performed in cultured human lymphocytes.
Source	:	Atofina, Paris-la-Défense, France.
Reliability	:	(1) valid without restriction
Flag	:	Material Safety Dataset, Critical study for SIDS endpoint

26.02.2004 (18)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	**rat**
Sex	:	female
Strain	:	Sprague-Dawley
Route of admin.	:	gavage
Exposure period	:	Gestation day 6 to 15.
Frequency of treatm.	:	daily
Duration of test	:	up to gestation day 20
Doses	:	50, 250 and 1000 mg/kg bw
Control group	:	yes, concurrent vehicle
NOAEL maternal tox.	:	= 1000 mg/kg bw
NOAEL teratogen.	:	= 1000 mg/kg bw
Method	:	OECD Guide-line 414 "Teratogenicity"
Year	:	1981
GLP	:	yes
Test substance	:	
Test substance	:	Test compound: TPS 32 Chemical name: di-t-dodecyl polysulfide CAS no.: 31565-23-8 Source: EAP Batch: 96000424 Sulfur content 31.10%
Method	:	Three groups of 25 mated female rats received the TPS 32 by oral gavage at the dose levels of 0, 50, 250 or 1000 mg/kg/day, each day from day 6 to day 15 post-coitum inclusive.

Clinical signs (including evidence of abortion/resorption) and mortality were checked daily. Food consumption and body weight were recorded at designated intervals during pregnancy.
On day 20 post-coitum, females were killed. The gravid uterus was weighed and fetuses were removed by hysterectomy. Females were examined macroscopically. Litter parameters were recorded: number of corpora lutea, implantation sites, resorptions, dead and live fetuses. The live fetuses were weighed, sexed, submitted to an external examination and then to soft tissue or skeletal examinations.

Result : No clinical signs, no unscheduled deaths, no abortions or total resorption were observed in any group.
The food consumption and body weight gain of the pregnant females from all treated groups were similar to those of controls.
No treatment-related macroscopic findings were observed, in any group. The post-implantation loss was similar in the 0, 50 and 250 mg/kg-day groups. In the 1000 mg/kglday group, a slightly increased post-implantation loss (represented mainly by late resorptions, observed in one female) was observed: it could not be demonstrated that this single event was treatment-related.
No treatment-related effects were observed on the number of live fetuses per animal, the fetal body weight or the sex-ratio.
No treatment-related external anomalies or malformations were observed in any group. No treatment-related soft tissue malformations or anomalies were noted in any group. No treatment-related skeletal malformations, anomalies or variations were observed in any group.

Conclusion : The No Effect Level was defined as 1000 mg/kg/day in terms of maternotoxicity, embryo-fetotoxicity and teratogenic effects.

Source : Atofina, Paris-la-Défense, France.

Reliability : (1) valid without restriction

Flag : Material Safety Dataset, Directive 67/548/EEC, Critical study for SIDS endpoint

26.02.2004 (19)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

(1) United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation, 2000. EPI Suite v 3.10 (April, 2001).

(2) Material Safety Data Sheet. TPS32, DITERTIODODECYL PENTASULPHIDE, CAS no. 68425-15-0. ATOFINA, 25/02/2003.

(3) Material Safety Data Sheet. TPS20, DITERTIODODECYL TRISULPHIDE, CAS no. 68425-15-0. ATOFINA, 25/02/2003.

(4) ATOCHEM. TPS 32, 1989.Evaluation en milieu aqueux de la biodégradabilité aerobie "ultime", Essai en fiole fermée.Centre d'application de Levallois, n° rapport:23736.

(5) ELF ATOCHEM S.A. TPS 32. Toxicité Aiguë vis-à-vis des Daphnies. Centre d'application de Levallois, Etude N°: 1209/98/A, le 9/07/98.

(6) ELF ATOCHEM S.A. TPS 32, Toxicitié vis-à-vis des Daphnies. Centre d'application de Levallois, Etude N°: 4352/96/A, le 19/12/1997.

(7) ELF ATOCHEM, Centre d'Application de Levallois, 1988.
TPS 32/TPS 27/TPS 20/TPS 37. Détermination de l'inhibition de la mobilité de Daphnia magna selon la norme AFNOR NFT 90301.

(8) ELF ATOCHEM S.A. TPS 32. Inhibition de la Croissance des Algues. Centre d'application de Levallois, N° d'étude BPL: 507/99/A, le 06/03/2000.

(9) IRCHA, 1989. Etude B.7102. Determination d'un Effet Inhibiteur de la Multiplication Cellulaire Bactérienne pour le produit TPS 32.
(unpublished report).

(10) Rapport Laboratoire Henri Lauressergues, Etude de la Tolérance chez l'Animal de trois Polysulfures, 4 Juillet 1973.

(11) SNEA(P) Test pour l'Evaluation de la toxicité aiguë par administration cutanée unique (DL50), chez le rat. Rapport Hazleton-IFT N° 606358 du 13.06.1986.

(12) SNEA(P) Test pour l'évaluation de l'irritation primaire et de la corrosion cutanées aigues, chez le lapin. Hazleton-IFT N°606332 du 07.06.1986,

(13) SNEA(P) Test pour l'évaluation de l'irritation et de la corrosion oculaires, chez le lapin. Hazleton-IFT N°606332 du 07.06.1986.

(14) SNEA(P) Test pour l'évaluation du pouvoir sensibilisant chez le cobaye. Hazleton-IFT rapport N°606332 du 07.06.1986.

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